Agilent
VnmrJ 3.2 Installation and Administration

User Guide

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VnmrJ 3.2 Installation

This chapter provides information on VnmrJ 3.2 installation requirements, installation procedures, installation options, software patches, and VnmrJ 3.2 restoration procedures. VnmrJ 3.2 installations are able to accommodate both Agilent and non-Agilent distributed systems with pre-configured Red Hat Enterprise Linux (RHEL) 5.X, 6.1.

| **NOTE** | After VnmrJ 3.2 installation, documentation is located in the VnmrJ 3.2 Help menu bar. |

| **NOTE** | For VnmrJ 3.2 Data Station installation information, see "VnmrJ 3.2 Offline Data Processing" on page 33. |

VnmrJ 3.2 Installation Requirements

Prior to VnmrJ 3.2 installation

- Verify that the firewall is disabled.
- Verify that SElinux is disabled.
- Verify that the console is connected and powered on.
- Verify that the network adapters are configured correctly. For more information, see *"Configuring Network Settings"* of the Linux for VnmrJ 3.2 User Guide.

NOTE	For pre-installed RHEL systems, the console connects to the external network card.

CAUTION	Firewalls and SElinux must be disabled for VnmrJ 3.2 installation.

Required items

- VnmrJ 3.2 Installation DVD
- Red Hat Enterprise Linux Installation DVD

VnmrJ 3.2 Installation

Table 1   VnmrJ 3.2 installation procedures

Section title	Description
Preinstallation-checking software packages	Install the VnmrJ 3.2 DVD to assess which RHEL Operating System (OS) software packages are needed.
Preinstallation-installing software packages	Install the RHEL Installation DVD to obtain needed RHEL OS software packages.
Installing VnmrJ 3.2 software	Install the VnmrJ 3.2 software.
Configuring acquisitions communications	Use the setacq command to establish communications between the host computer and the NMR console.
Creating the acqproc user	Use the aqcqproc command to turn on/off information exchange between the host computer and the NMR console.
Configuring system settings	Configure VnmrJ 3.2 using the VnmrJ 3.2 System Settings window.
Setting the lock frequency	Set the lock frequency on the system after VnmrJ 3.2 and the magnet are installed.
Configuring proton experiments	Configure VnmrJ 3.2 Proton Experiments using the Proton Experiments menu.

Preinstallation-checking RHEL software packages

The initial phase of installation checks the RHEL OS for software packages required to install and run VnmrJ 3.2. If additional software packages are required, a message box displays, indicating that the RHEL installation DVD is needed. If no additional software packages are required, the Installation window will appear.

With Linux 5.x, removable media, CDs and DVDs, are mounted. Executing programs or scripts directly from the CD/DVD is not permitted. Double-clicking on the load.nmr icon will fail.

NOTE	Users must be logged in as root. If the user is not root, "su" to root.

1 Insert the VnmrJ 3.2 DVD.

2 A window displays after the DVD has been mounted by the system. Note the title bar, this is the DVD name. Use this name in the following step.

3 Change to the DVD directory and start the Installation by entering the following in a terminal window.

    a `cd /media/`*DVD_Name*
      for example:
      `cd /media/VnmrJ_3.x`

    b `sh ./load.nmr`

4 Click **Continue** in the message box.
If software packages are needed, a message box displays indicating that the RHEL Installation DVD may be required.

5 Click **OK** and continue to "Preinstallation–installing software packages".

6 If no additional software packages are needed, continue to "Installing VnmrJ 3.2 software".

Preinstallation—installing software packages

NOTE	Users must be logged in as root. If the user is not root, "su" to root.

1 Eject the VnmrJ 3.2 DVD in a terminal window:

    a `cd /`

    b `eject`

2 Insert the RHEL Installation DVD and a the terminal window, type:

`cd /tmp/preinstall`

3 Wait for the DVD to be auto-mounted by the system and in the terminal window, enter:

```
./installpkgs
```

Installing packages may take a few minutes.

4 Eject the RHEL Installation DVD:

```
eject
```

5 Continue to "Installing VnmrJ 3.2 software".

Installing VnmrJ 3.2 software

| NOTE | Users must be logged in as root. If the user is not root, "su" to root. |

1 Insert the VnmrJ 3.2 DVD.

2 A window will appear after the DVD has been mounted by the system. Note the title bar, this is the DVD name. Use this name in the following step.

3 Change to the DVD directory and start the installation by entering the following in a terminal window.

   a `cd /media/`*DVD_Name*
     for example:
     `cd /media/VnmrJ_3.x`

   b `sh ./load.nmr`

4 The Load VnmrJ Software will appear. Select the correct system for your installation.

5 Configure the VnmrJ 3.2 installation options. For more information, see "VnmrJ 3.2 Systems-Installation Options" on page 21.

400-MR DD2 system—VnmrJ 3.2 installation window
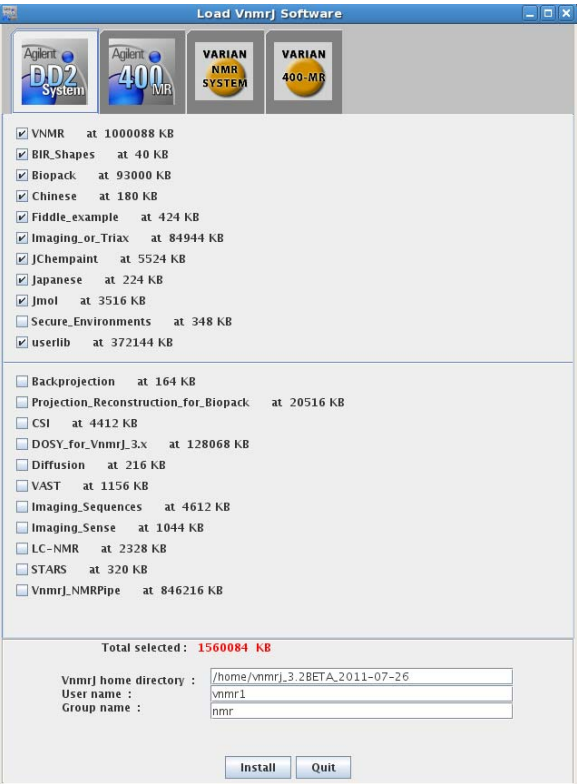
DD2 MR system—VnmrJ 3.2 installation window

400-MR system—VnmrJ 3.2 installation window   VNMRS system—VnmrJ 3.2 installation window

6 Click **Install**.

7 After VnmrJ 3.2 installation is complete, VnmrJ 3.2 Administration will open.

8 If you are upgrading your software, update users in VnmrJ 3.2 Administration.
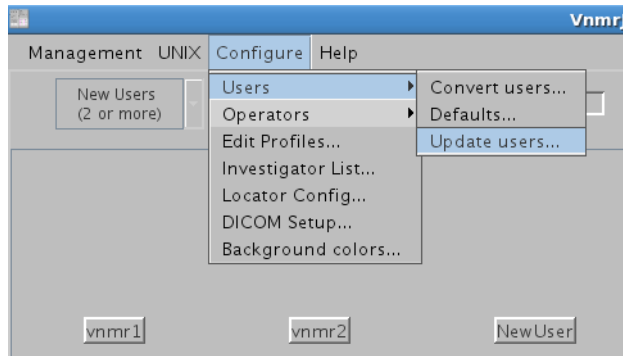
a Go to **Configure > Users > Update Users**.
The Update VnmrJ Users window displays with user accounts listed on the left side of the window.
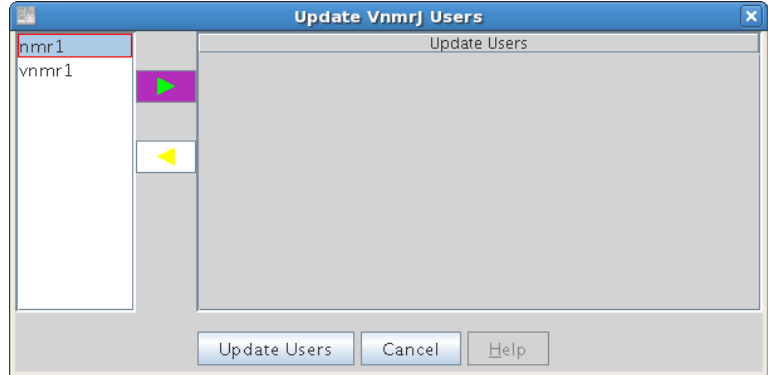
b Select the accounts to be updated.

Hold the Control and Shift keys to select multiple accounts with the same interface.

c Click the highlighted, green arrow to move the accounts to Update Users.

      d Click **Update Users**.
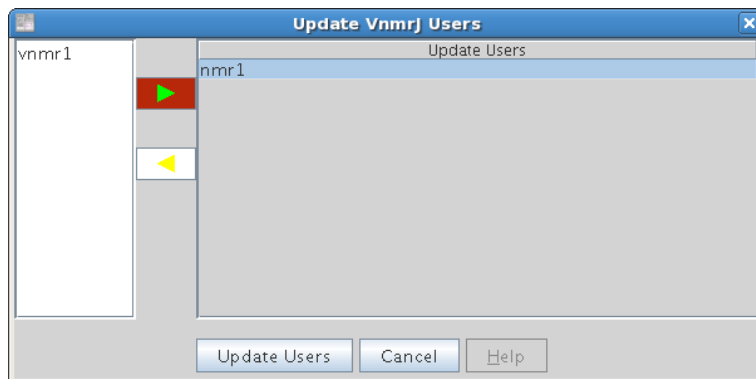
9 Continue to "Configuring acquisitions communications".

10 Close the VnmrJ 3.2 interface that has popped up.

NOTE   VnmrJ 3.2 automatically installs "vnmr1" as the administrator.

Configuring acquisitions communications

This section describes how to use the setacq command to establish communications between the host computer and the NMR console. Skip this section if VnmrJ 3.2 is for a data station.

The default admin user is "vnmr1". For new installations, there is no password. To add or change the admin password, use standard Linux tools. For upgrade installations, after running Update Users the previous admin login will be retained. See "Installing VnmrJ 3.2 software"step 8.

NOTE   Users must be logged in as root. If the user is not root, "su" to root.

1 After installing VnmrJ 3.2 software, reboot the system (**System > Shutdown > Restart**).

2 Log in as the administrator, typically vnmr1.

3 Run setacq by entering the following commands in a terminal window:

```
# cd /vnmr/bin
```

```
#./setacq
```

CAUTION	Do not reboot or reset the NMR console until setacq has finished. The process may take eight or more minutes.

4 Expproc will start and stop as needed.

5 Wait for setacq to finish the update process.

6 Wait for the following message:

"**Starting Acquisition communications**"

7 Reboot the system (**System > Shutdown > Restart**).

Creating the acqproc user

Daemons, known as the proc-family, direct communications between the host computer and the console on systems that include a magnet installation (spectrometers systems, not data stations).

Create the user acqproc as follows:

1 Log in as **root**.

2 Enter the following command:

```
# /vnmr/bin/makesuacqproc
```

3 All users can enable or disable the daemons once acqproc is created by entering the following command:

```
user> su acqproc
```

4 Log in as vnmr1.

Install VnmrJ 3 patches if needed.

For more information, see "VnmrJ 3 Patches".

5 Launch VnmrJ 3.2 software by double-clicking the VnrmJ 3 icon on the desktop.

Configuring system settings

After VnmrJ 3.2 is installed, configure the system by using the VnmrJ 3.2 System Settings window. Typically, "vnmr1" is set as the VnmrJ 3.2 administrator.

1 Log in as the administrator.

2 Start **VnmrJ**.

3 Click **Edit > System settings**.

The System Settings window has two tabs: **System** and **Display/Plot**.

4 Configure system settings for the spectrometer system.
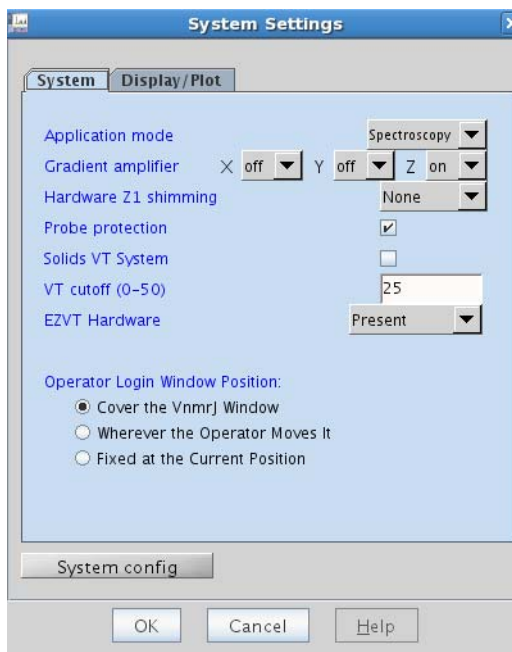
Figure 1   System settings window

Table 2   System setting

Tab	Fields
System	• Application mode—Spectroscopy, LC-NMR. • Gradient amplifier-on/off selection for each installed gradient axis. • Hardware Z1 shimming-none for no Z1 shimming, Delay for Z1 shimming enabled during delay time, or Presat for Z1 shimming enabled during delay time preceding presat. • Probe protection-check to enable. • VT cutoff (0-50)-specify VT cutoff temperature; 25 ºC recommended. • EZVT Hardware-select appropriate setting. • Operator Login Window Position-select appropriate setting.
Display/plot	• Set display from plotter aspect ratio (`wysisyg`)-select to enable. • Spectrum updating during phasing (0-100)-set the percentage of the display that is updated during interactive phasing. 100 is recommended. • Max # of pens-number of plotter pens to use. • Show Tooltips-select to enable. • Max # of items to show in Locator-set the number of locator items to show. A Setting greater than 2000 starts to diminish the performance. • Display only matching items in locator-select to enable. • Process data on drag-and drop from locator-select to enable.

Resetting the lock frequency

Superconducting magnets drift, and periodically the spectrometer's lock frequency (lockfreq) will need to be reset.

1 Write down the spectrometer's current lock frequency. The lockfreq is available in the System Configuration window (**Edit > System Settings > System config**).

It can also be obtained by entering `lockfreq?` in the VnmrJ command line.

2 Use a water sample. Such as doped 1% H^2O in D^2O or AutoTest samples.

3 Use a water sample such as the AutoTest sample or 1% H_2O in D_2O.

NOTE	Imaging systems should use tap water or water/$CuSO_4$.

4 Load a proton experiment from the Experiment menu.

   a Set the solvent to D_2O.

   b Set sw=5e6, nt=1 ss=1, gain=20, and spin=0.

   c Set z0=0.

NOTE	For Imaging systems, set all shims to **0** by loading the **reg0** shim set from /vnmr/shims.

5 Acquire a spectrum.

6 Expand the region around the water peak.

7 Place the cursor on the water peak.

8 In the VnmrJ command line:

   a enter `nl`

   b then enter `movetof`

9 Acquire another spectrum.

10 Place the cursor on the water peak, and enter `setlockfreq` in the VnmrJ command line.

This will reset the lock frequency. The system will lock with z0 near 0. If you are vnmr1, check that the new lockfreq value is in the config file.

Alternate method

The lock frequency can also be reset by entering new
`lockfreq` values until z0 is at the desired value. This is
done in the VnmrJ command line.

1 Write down the spectrometer's current lock frequency.
The lockfreq is available in the System Configuration
window (**Edit > System Settings > System config**).
It can also be obtained by entering `lockfreq?` in the
VnmrJ command line.

2 In the VnmrJ command line, enter:
`lockfreq=xxxxxxxx su`
where "xxxxxxxx" is a new lock frequency value.
While differences of a few hundred Hz in the final value
are not critical, the lock frequency should be entered to
the tenth of a Hz resolution; seven places to the right of
the decimal.
For example: `lockfreq=61.38520001`.

3 Lock the sample to find z0.

4 Continue the above steps until z0 is at the desired value.

Configuring proton experiments

1 Log in to VnmrJ 3.2 as the administrator.

2 From the **Experiment** menu, click **Proton**.

3 From the **Start** tab, click **Shim**.

4 In the File box, type "`reg0`".

5 Click the **Setup Hardware** button.

When the message **"Setup complete"** appears, the system is
ready.

VnmrJ 3.2 Systems-Installation Options

VnmrJ 3.2 offers general and password configuration options to be installed with VnmrJ 3.2.
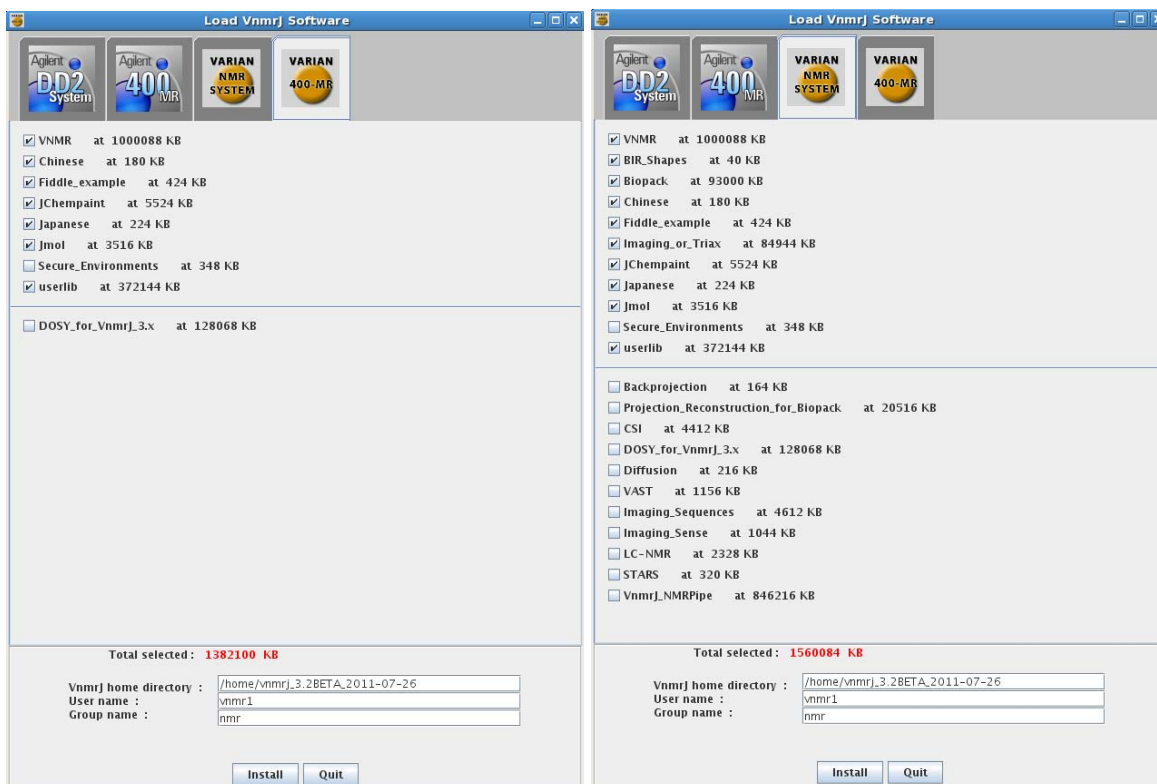

400-MR DD2 system—VnmrJ 3.2 installation window   DD2 MR system—VnmrJ 3.2 installation window
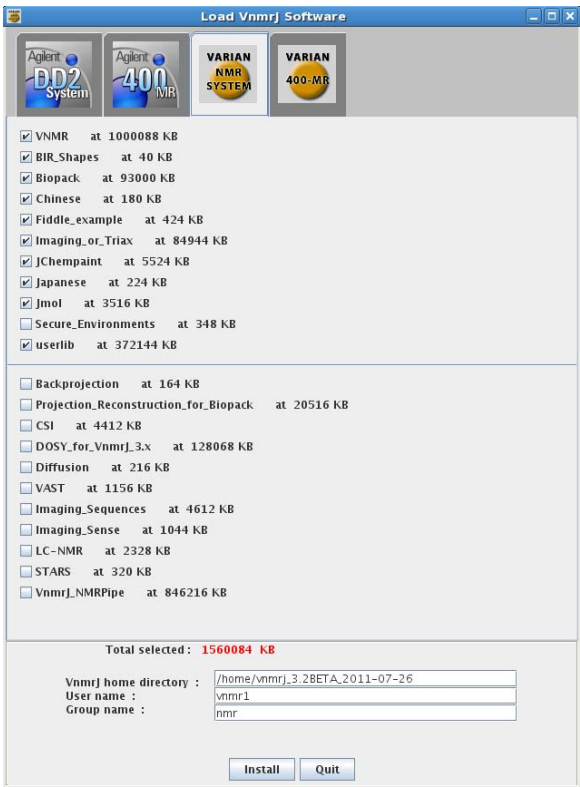
400-MR system—VnmrJ 3.2 installation window   VNMRS system—VnmrJ 3.2 installation window

General installation options for DD2 MR and VNMRS systems

The following is a list of general options and descriptions. Select the check box next to each option you want to load.

Table 3   Installation options for DD2 MR and VNMRS systems

Option	Description
VNMR	Loads the standard VnmrJ 3.2 and VNMR software.
BIR_Shapes	Loads the B1 Independent Rotations (BIR4) pulse shapes.
Biopack	Loads Biomolecular NMR software.
Chinese	Loads the Chinese language support.
Fiddle_Example	Loads an example dataset for Fiddle Reference deconvolution.
Imaging_or_Triax	Loads Imaging or Triple-Axis gradient software.
JChemPaint	Loads the integrated JChemPaint molecular editing software.
Japanese	Loads the Japanese language support.
Jmol	Loads the integrated Jmol molecular viewing software.
Secure_Environments	Option enhanced with security features, validation features, audit trails, and other tools to help facilitate compliance with regulations associated with electronic record authenticity.
userlib	Loads the user-contributed library.

Password-requiring options for DD2 MR and VNMRS systems

Table 4 lists the password-requiring options and descriptions. A password field is visible when the option is selected. Enter the password in the field, passwords are case-sensitive. The list of options presented is system dependent.

VnmrJ passworded options can be installed by the administrator after installation in the VnmrJ command line.

1 Enter **vnmrjOptions** in the VnmrJ command line.

2 Enter the password for the desired options on the VnmrJ Options Installer popup window.

Table 4   Password required options

Option	Description
Backprojection	Loads the Backprojection software.
Projection_Reconstruction_for_Biopack	Loads the Projection_Reconstruction_for_Biopack software.
CSI	Loads the Chemical Shift Imaging software.
DOSY_for_VnmrJ_3.x	Loads High-Resolution Diffusion-Ordered Spectroscopy for VnmrJ 3.2 software.
Diffusion	Loads the Diffusion software.
VAST	Loads the VAST software.
Imaging_Sequences	Loads Imaging_Sequences software.
Imaging_Sense	Loads Imaging_Sense software.
LC-NMR	Loads Liquid Chromatography NMR software.
STARS	Loads the Spectrum Analysis of Rotating Solids software.
VnmrJ_NMRPipe	Loads the VnmrJ NMR Pipe software.

General installation options for 400-MR DD2 and 400-MR systems

The following is a list of general options and descriptions. Select the check box next to each option you want to load.

Table 5   Installation options for 400-MR DD2 and 400-MR systems

Option	Description
VNMR	Loads the basic VnmrJ 3.2 and VNMR packages.
Chinese	Loads the Chinese language support.

Table 5   Installation options for 400-MR DD2 and 400-MR systems

Option	Description
Fiddle_Example	Loads an example of fiddle reference deconvolution.
JChemPaint	Loads the integrated JChemPaint molecular editing software.
Japanese	Loads the Japanese language support.
Jmol	Loads the integrated Jmol molecular viewing software.
userlib	Loads the user-contributed library.

Password-requiring options for 400-MR DD2 and 400-MR systems

The following is a list of options (and descriptions) that require a password. A password field is visible when the option is selected. Enter the password in the field (passwords are case-sensitive). The list of options presented is system dependent.

Table 6   Password required options

Option	Description
DOSY_for_VnmrJ_3.x	Loads the DOSY for VnmrJ 3.2 software.

Spectrometer configuration

Use the Spectrometer Configuration window to configure the NMR spectrometer hardware.

1 Log in to the system as the administrator.

2 Launch VnmrJ.

3 Click the **System config** button in the System Settings window.

A Spectrometer Configuration window similar to Figure 2 opens.
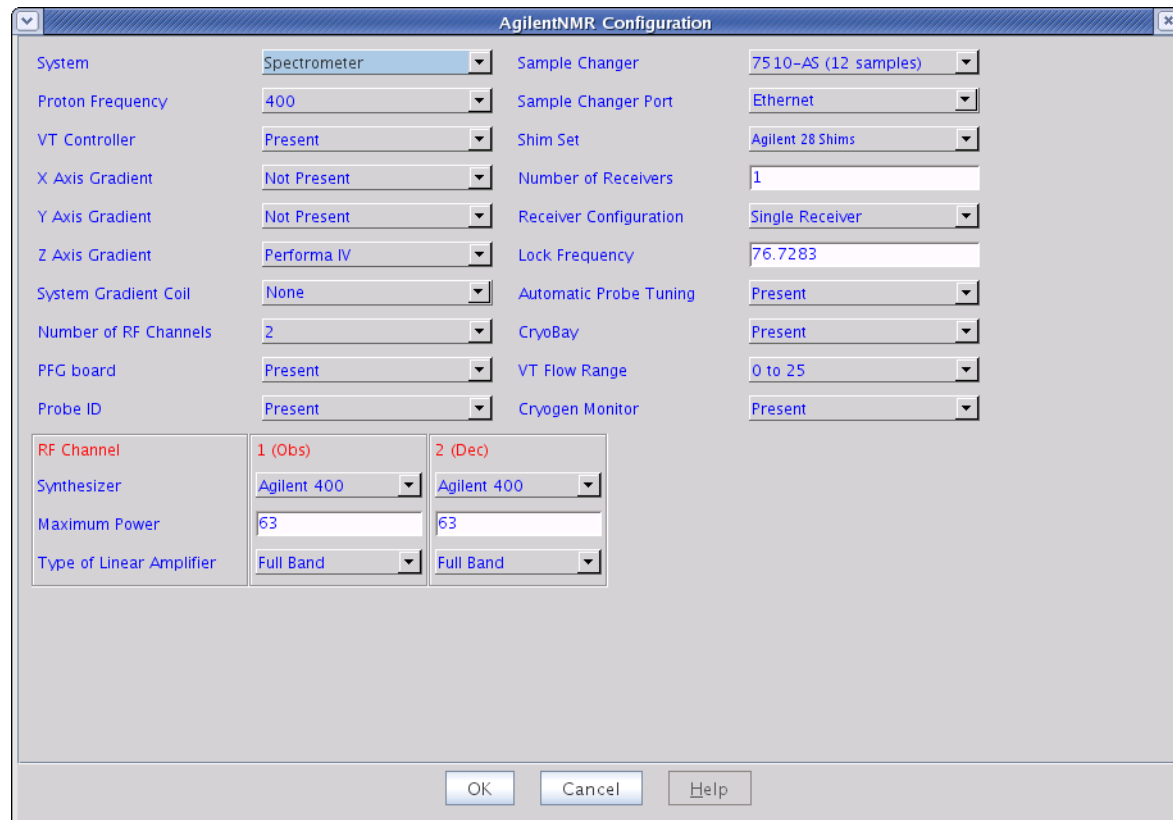
Figure 2   Spectrometer configuration window

4   Check that the configuration values are correct for your system.
    Refer to Table 7 General Configuration for more information on these values.

5   Configure each RF channel.
    Refer to Table 8 RF Channels Configuration for information on each selection.

6   Click **OK** to save the system settings or **Cancel** to make no changes and close the System Settings window.

7 Exit and restart VnmrJ 3.2 to enable the acquisition features in the main menu if the system is changed from a data station to a spectrometer.

Table 7   General configuration

Label	Choices	Explanation
System	Spectrometer, Data Station	Set whether the function of the workstation is to control a spectrometer or to operate as a separate data station. If Data Station is selected, VnmrJ 3.2 does not allow acquisitions (the go command, its aliases, and related commands do not work).
Proton frequency	85, 100, 200, 300, 400, 500, 600, 700, 750, 800, 900, 3T, 4T	Set ^{1}H frequency for spectrometer-type systems.
VT controller	Not Present, Present	Set whether a VT controller is present.
X axis gradient, Y axis gradient, Z axis gradient	Not present, Gradient coordinate Rotator Performa I, Performa IV, Performa XYZ, Homospoil	Set appropriate values for installed gradient amplifier.
System gradient coil	Enter value.	Fill in the value for the current system gradient coil (`sysgcoil`).
Number of RF channels	1, 2, 3, 4, 5	Set number of RF channels available (the lock channel is not included).
PFG board	Present, Not Present, Microimaging	Present—Select if there is only a PFG controller board. Not Present—Select if there is only a gradient controller board. Microimaging—Select if there is both a PFG and gradient controller board.
Sample changer	None, Carousel, SMS 50 Sample, SMS 100 Sample, VAST, NMS, LC-NMR, 768 AS, 7510-AS, 7600-AS	Set the type of optional sample changer. Select **None** if no sample changer is present or to disable an attached sample changer. For more information, see Chapter 6, "Automated Hardware".
Sample changer port	None, Com1, Ethernet	Set communications port used for the sample changer. Select **Not Used** if no sample changer is present.

Table 7   General configuration (continued)

Label	Choices	Explanation
Agilent 28 Thin Shims	Agilent.13.Shims, Agilent.14.Shims, Agilent.15.Shims, Oxford.15.Shims, Oxford.18.Shims, Agilent 18.Shims, Agilent 20.Shims, Agilent 23.Shims, Agilent 26.Shims, Agilent 27 Shims Agilent 27 Shims: high power Agilent 28.Shims, Agilent 28 Shims: high power Agilent 29.Shims, Agilent 35.Shims, Agilent 40 Shims, Agilent 40 Shims: high power Ultra 18 Shims, Ultra 39 Shims, Whole Body Agilent Combo Shims Agilent 28 Thin Shims Agilent 28 Thin Shims: high power	Set the type of shims on the system.
Number of receivers	Enter value.	Enter the number of receivers installed on the system.
Receiver configurations	Single receiver Parallel Multi nuclear	Single receiver—standard receiver configuration. Parallel—Imaging multi-receiver configuration. Multi nuclear—for Liquids two-receiver systems.
Lock frequency	Enter value.	Enter the value of lock frequency in MHz. It is recommended to set the lock frequency to 0.1 Hz, with "9999" as the last four digits. For example, the lock frequency value for a 500 MHz system may be "76.3249999".
Automatic probe tuning	Present, not present	Select **present** if ProTune hardware is installed and in use, see also "Setting Up Automatic Probe Tuning" on page 101.
CryoBay	Present, not present	Select **present** if CryoBay hardware is installed and in use.

Table 7   General configuration (continued)

Label	Choices	Explanation
VT Flow Range	0 to 25, 0 to 50	Set according to the flow range available to the flow monitor.
Cryogen Monitor	Present, Not Present	Select present if cryogen monitor hardware is installed.

Table 8   RF channels configuration

Label	Choices	Explanation
Synthesizer	None, PTS320, PTS500, PTS620, PTS1000, Direct Digital, Direct Digital II	Set the type of frequency synthesizer.
Maximum power	Enter value.	Set the maximum power (upper limit) to the current RF channel to prevent damage from high power RF. The recommended value is **63**.
Type of linear amplifier	Full band, Low band, Broadband Shared	Select **Full band** for DD2, 400-MR DD2, VNMRS, and 400-MR systems.

VnmrJ 3 Patches

The latest VnmrJ 3 patches can be downloaded from the Agilent NMR Software Corner, http://www.chem.agilent.com/EN-US/Support/Pages/nmrsoftwarecorner.aspx.

Check the patch level

1 Log in as vnmr1.

2 Open a terminal window and type:

```
vnmr1> ls /vnmr/adm/patch
```

3 The installed patches are listed.
The system returns "**No such file or directory**" if no patches are listed.

Download and install a patch

1 Log in as vnmr1.

2 Go to http://www.chem.agilent/EN-US/Support/Pages/NMRPatches.aspx.

3 Navigate to the Software Patches page and find the appropriate patch.

4 Read the Readme file for the patch before downloading and installing the patch.
Any patch specific instructions are specified in this file.

5 Follow the instructions in the Readme file.

6 Click the patch name to download it.

Use the patchinstall script to install the patch (as specified in the Readme file).

Restoring VnmrJ 3.1 after Installing VnmrJ 3.2

1 Switch the link /vnmr to VnmrJ 3.1. As root, enter:

```
rm /vnmr
```

2 Confirm removal of symbolic link by entering "y", as shown below.

```
rm: remove symbolic link `/vnmr'? y
```

3 Establish symbolic link to VnmrJ 3.1 by entering:

```
ln -s /home/vnmrj_3.1_A /vnmr
```

4 To confirm the restored link, enter:

```
ls -l /vnmr
```

The following output will be displayed:

lrwxrwxrwx 1 root root 20 Feb 6 09:14 /vnmr -> /home/vnmrj_3.1_A

5 Reset the master controller.

6 Run setacq.

7 Run dbsetup.

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VnmrJ 3.2 Offline Data Processing

This chapter provides installation information for VnmrJ 3.2 Offline Data Processing (ODP). ODP enables users to view and analyze Agilent NMR data on Mac or Windows operating systems.

| NOTE | To add VnmrJ 3.2 password-protected options, see "VnmrJ 3.2 Systems-Installation Options" on page 21. |

System Requirements

Host computers with Linux OS

- Dell Optiplex 755N (Red Hat Enterprise Linux 5.1)
- Dell Precision 390N (Red Hat Enterprise Linux 5.1)
- Dell Precision T3400 (Red Hat Enterprise Linux 5.1)
- Dell Precision T3500 (Red Hat Enterprise Linux 5.3)
- Hewlett-Packard Z400 (Red Hat Enterprise Linux 6.1)

ODP on Windows OS

- Windows XP Professional, 32-bit
- Windows 7 Enterprise, 64-bit, with or without SP1
- Windows 7 Ultimate Edition, 64-bit, with or without SP1

ODP on Mac OS

- Mac OS X 10.6 Snow Leopard
- Mac OS X 10.7 Lion

VnmrJ 3.2 Windows ODP Installation

VnmrJ 3 DataStation supports

- Windows XP Professional, 32-bit
- Windows 7 Enterprise or Ultimate Edition, 64-bit

NOTE   VnmrJ Imaging is not available for Windows VnmrJ 3.2.

Install

1 Insert the VnmrJ 3 DataStation DVD.

2 Click **Next** on the initial installation window to begin the installation setup process.

3 Accept the terms of the license agreement and click **Next**.

4 Enter Customer Information and click **Next**.

5 Select the Setup Type and click **Next**.

6 Review the Prerequesite and Selected features to be installed and click **Next**.

7 Click **Install** to begin installation. Click **Back** to review or change installation settings before clicking Install.

8 Installation will begin.

9 After installation has completed, the InstallShield Wizard will prompt you to restart your computer.

CAUTION   System must be rebooted after completion of VnmrJ 3.2 installation.

To access the installed VnmrJ 3 DataStation:
Start > All Programs > Agilent VnmrJ 3 DataStation.

Modify

Modify VnmrJ 3 DataStation in Add or Remove Programs: **Start > Control Panel > Add or Remove Programs.**

1 Select VnmrJ 3 DataStation from the list of Currently installed programs, and click **Change**. The InstallShield Wizard will display.

2 Select **Modify** and click **Next**.

3 Select additional features to install and click **Next**.

4 Review features to be installed and click **Next**.

5 Click **Install** to begin installation. Click **Back** to review or change installation settings before clicking Install.

6 Installation will begin.

7 After installation has completed, the InstallShield Wizard will prompt you to restart your computer.

Repair or maintenance

Repair VnmrJ 3 DataStation in Add or Remove Programs: **Start > Control Panel > Add or Remove Programs.**

1 Select VnmrJ 3 DataStation from the list of Currently installed programs, and click **Change**. The InstallShield Wizard will display.

2 Select **Repair** and click **Next**.

3 VnmrJ 3 DataStation Maintenance procedures will begin.

4 After maintenance has completed, click **Finish**.

Remove

Remove features in Add or Remove Programs:
Start > Control Panel > Add or Remove Programs.

1 Select VnmrJ 3 DataStation from the list of Currently installed programs, and click **Remove**. The InstallShield Wizard will display.

2 Select **Remove** and click **Next**.

3 Select the features for removal and click **Next**.

4 Confirm the uninstall by selecting **Yes**.

VnmrJ 3.2 ODP Mac Installation

VnmrJ 3 DataStation supports

- Mac OS X 10.6 Snow Leopard
- Mac OS X 10.7 Lion

Java package

The Java package is not installed with Mac OS X Lion.
To download the Java package:

1 In a terminal window, enter `java`.

2 Follow the operating system instructions to download the package.

C Compiler

For tasks that require a C Compiler, download the free Xcode package from the Mac App store.

A C Compiler is required when working with pulse sequences and other operations.

ImageMagicK

For certain printing tasks, such as the "Print Screen..." option, tools from the free ImageMagicK package are used. If this package is not installed on your system, it can be downloaded from the www.imagemagick.org site.

Adding user accounts

NOTE	Disable the password request from `sudo` before adding user accounts.

1 To disable the password request from `sudo`, enter the following in a shell tool:

```
sudo -e /private/etc/sudoers
```

2 Change the following line, near line 34, from:

```
%admin    ALL=(ALL) ALL
```

to

```
%admin    ALL=(ALL) NOPASSWD: ALL
```

3 Use standard MacOS tools to create additional user accounts.

4 Use VnmrJ Admin to enable VnmrJ for those accounts.

5 To re-enable the password, undo the change that added the NOPASSWD: field.

Install

The VnmrJ Installation package is installed in the **/Applications/VnmrJ32A.app** directory. A link is made from **/vnmr** to the appropriate subdirectory of **/Applications/VnmrJ32A.app**. The **/vnmr/bin/makeuser** script is automatically executed. It creates a vnmrsys subdirectory in the HOME directory of the installer. The VnmrJ installation does not change dot-files in the user's home account.

Start the VnmrJ application as you would any other Mac application. The VnmrJ32A.app can also be placed on the dock for quick access.

Updating the PATH parameter

To run VnmrJ, seqgen, or other VnmrJ commands from a terminal window, the PATH parameter must be updated to include **/vnmr/bin**.

To update the PATH parameter, add the following line to a ".cshrc" file:

```
source /vnmr/user_templates/.vnmrenvsh
```

Installing VnmrJ

1 Insert the VnmrJ 3 DataStation DVD.

2 Change to the mac subdirectory and select the VnmrJ Installer ".pkg" file.

3 The Mac VnmrJ 3.2 Datastation Installation window will display.

Figure 3   Mac VnmrJ 3.2 Datastation installation

4 Click **Continue**.

5 Read the Important Information and click **Continue**.

6 Read the Software License Agreement, click **Continue** and **Agree**.

7 Click **Install** to begin installation.

8 After installation, a Summary screen will display.

To access the installed VnmrJ 3 DataStation:
Applications > VnmrJ32A.app.

Troubleshooting Tip

On some systems, after installing VnmrJ, the application will start but VnmrJ menus and panels may not be populated. The problem is related to various networking configurations. The solution is to add your systems hostname to the `/etc/hosts` file.
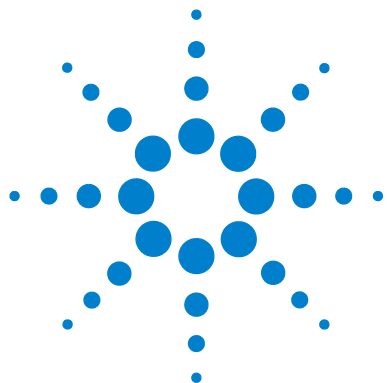
If you need to do this, use the command

`sudo vi /etc/hosts`

and append your hostname to the `127.0.0.1 localhost` line if your system is on DHCP or is not networked.

If your system has a fixed IP address, add your IP address and hostname on a new line in the `/etc/hosts` file.

3
VnmrJ 3.2 Administration

This chapter describes VnmrJ 3.2 administration procedures, administrative functions, and account administration.

Agilent Technologies

Agilent NMR Software Corner on the Web

The NMR Software Corner offers the following information for registered VnmrJ 3.2 users:

- Software patches
- Online manuals
- Agilent MR and MRI News - current issue and searchable archive
- User library - also provides additional software such as BioPack
- Magnetic Moments newsletter archive
- Upgrade information
- FAQs
- Bug lists

Registering for Software Corner access

Use the following procedures to register as a VnmrJ 3.2 user:

1 Register as a VnmrJ 3.2 user to be eligible to access the User Pages.

2 Click **Registration Form**.

3 Fill in the form and click **Submit**.

Starting the VnmrJ 3.2 Admin Interface

1 If the current user is the administrator, click the VnmrJ 3.2 Admin icon on the desktop and log in to the workstation using the VnmrJ 3.2 administrator login.

2 If the current user is not the administrator, open a terminal window and change users to the VnmrJ 3.2 administrator account.

Enter `vnmrj admin` at the prompt.

3 If prompted, enter the administrator password to start VnmrJ 3.2 Admin; see Figure 4.
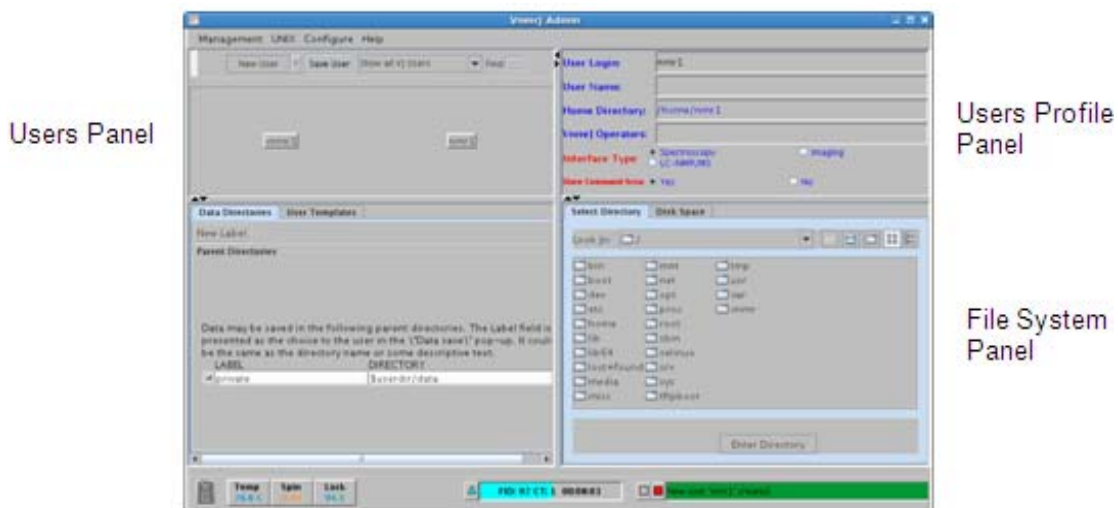
Figure 4   VnmrJ 3.2 administrator window

VnmrJ 3.2 Admin Interface

The VnmrJ 3.2 Admin interface provides the tools for administering VnmrJ 3.2 software and user accounts, see Figure 4. Select Administration functions from the menu bar.

Table 9   VnmrJ 3.2 Admin menu

Menu item	Description
Users	Displays users in the users panel and makes available all the administrative functions, see "User Account Administration" on page 49.
Printers	Displays printer functions using pop-up window, see Chapter 5, "Configuring Printers for VnmrJ 3.2".
Cost/Time accounting	VNMR ACCOUNTING window. See VnmrJ 3.2 Accounting Administration.
Console display sharing	Turns on sharing of display 0 for virtual network connections.
Exit	Exits and closes VnmrJ 3.2 Admin.

Table 10   UNIX menu

Menu item	Description
File system	Pop-up window displays file system information; see "Viewing the File System" on page 84, for more information and instructions.
Command window	Opens an operating system terminal window.

Table 11   Configure menu

Menu Item	Description
Users	Select additional functions using pop-up windows: • Convert users-opens the Change vnmr users to VnmrJ 3.2 user window. See "Converting user accounts to VnmrJ 3.2" on page 55. • Defaults-opens the default values window. See "User account defaults" on page 58. • Update users-opens the Update VnmrJ 3.2 Users window. See "Updating user accounts" on page 56.
Operators	• Edit operators-opens the Modify Operators window (Modify Operators tab). See "Adding Operators to a User Account" on page 64. • Delete operators-opens the Modify Operators window (Delete Operator tab). See "Deleting Operators from User Accounts" on page 81. • Reset password-opens the Reset Operators Password window. See "Resetting Operator Password" on page 74. • Preferences-opens the Preferences window for setting the default operators password and for selecting a default login icon. See "Setting Operator Default Password" on page 73.
Automation	Calls the Automation Configuration pop-up window.
Edit profiles	Creates and assigns user profiles containing the protocols, rights and tools. See "Creating, Editing, Viewing, and Deleting Profiles" on page 68.
Investigator	Lists Enter investigators in the pop-up window.
Background colors	Changes the default background colors of the VnmrJ 3.2 Admin windows.

Table 12   Help menu

Menu item	Description
VnmrJ 3.2 help	Opens the VnmrJ 3.2 HTML help pages in a browser.
Admin help	Opens the VnmrJ 3.2 Administration HTML help pages in a browser.
Online manuals (PDF) ...	Opens the VnmrJ 3.2 online manuals in PDF format.

User Account Administration

User accounts are created or set up using the VnmrJ 3.2 Admin interface. You can use the VnmrJ 3.2 interface to set up new accounts and configuration, assign a group of operators to a single user account.

VnmrJ 3.2 interfaces

Each VnmrJ 3.2 account can be set up with an interface and appropriate privileges. The main interfaces are listed in the below table.

Table 13   VnmrJ 3.2 interface menu

Interface	Description
Spectroscopy	The spectroscopy interface is designed for both automated and manual operation, with or without a sample changer. There can be two types of users of the spectroscopy account- the account owner and the operator.
Account owner	The account owner is the operating system (OS) login user, and therefore, the owner of the account and any acquisitions and data while logged in. The VnmrJ 3.2 login window (if displayed) sets the operator parameter and other properties set by VnmrJ 3.2 Admin, such as the user profile, panellevel, etc. The account owner sets up the preferences and settings of the account.
Operator	The operator is a user of the account but is not the OS login user of the account, therefore, does not own any of the files in the account. The operator has VnmrJ 3.2 access via a name and password entered on the VnmrJ 3.2 login window and can operate the software.
Imaging	The imaging interface provides the user with the full range of functions necessary for the acquisition of MRI data, the design of imaging sequences, building study protocols, and processing of imaging data.

Creating a single new user account

Use this procedure to create a single new user account. New user accounts will contain default values set in User Account Defaults, see "User account defaults" on page 58. To create multiple new user accounts, see "Creating multiple new user accounts" on page 51.

1 Select **Management**.
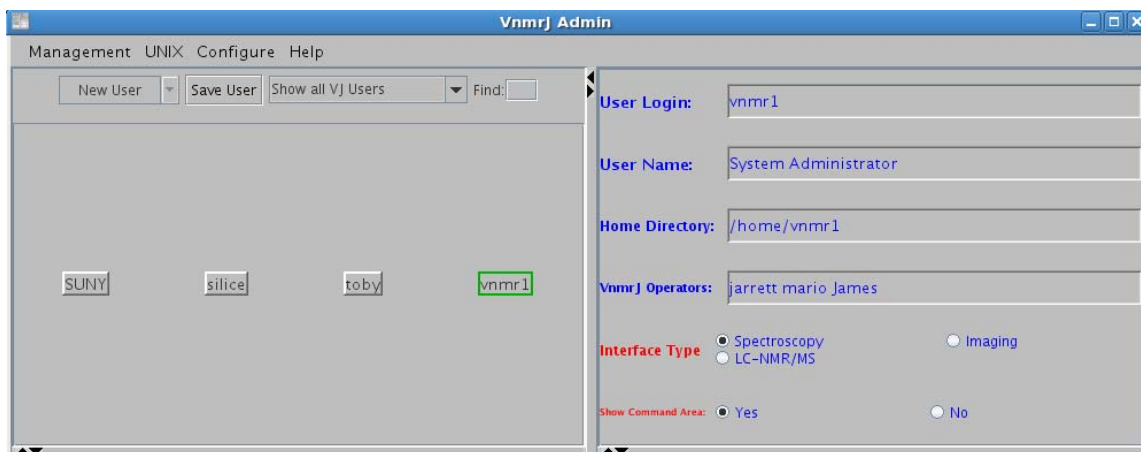
Figure 5   VnmrJ 3.2 admin window

2 Select **Users**.

3 Select **Show all VJ Users**.

4 Click **New User**.

New User appears with a box around it and the account's profile is displayed in the User Profile Panel.

5 Fill in the **User Profile Panel** as appropriate.

The User Profile Panel (by default) has five sections. See "User account defaults" on page 58 to view other fields, data dir, and so on.

Field	Description
User login	Type login name and select **TAB**. Prompt is displayed in the user login field.
User name	Optional. Enter a user name.
Home directory	New users with no operating system account:
	Setup is automatic and applies the user defaults (see User Account Defaults).
	Current users with an operating system account:
	The user's operating system account home directory is used.
VnmrJ 3.2 operators	Optional. List other users with VnmrJ 3.2 operation privileges.
Interface type	Click the **Option** button to select the interface type, See "VnmrJ 3.2 interfaces" on page 49.

6 Click **Save User**.

Creating multiple new user accounts

Use this procedure to create multiple new user accounts. The new user accounts will contain default values set in User Account Defaults, see "User account defaults" on page 58. To create a single new user account, see "Creating a single new user account" on page 50.

1 Select **Management** from the main menu bar.

2 Select **Users**.

3 Click the **New User** arrow.

4 Select **Multiple Users** from the drop-down menu.

5 Click **New Users (2 or more)**.

The Create 2 or more users window opens.

6 Enter the **login name** for each user. Separate each user name by a space.

7 Select the interface assigned to the multiple users. See

8 Click **Update Users**.

The home directory is automatically setup (new users - no operating system account) based upon the user defaults (see). Or if the user was first set up as an operating system account, the user's operating system account home directory is used.

Using a .csv file to add users

1 The .csv file's comment lines must start with a number.

2 In the first line, enter a list of column keywords separated by commas. The only required columns are login and itype. Column keywords can be listed in any order on the first line. List subsequent lines of values, separated by commas, in the same order as the column keywords listed on the first line.

Column keyword	Description
login	required-user login
itype	required-Spectroscopy or Imaging

Column keyword	Description
name	full name or description
home	home directory for user
email	user email address
profile	basic liquids, all liquids, common liquids, all imaging

Default user information will be used for Information not defined in the .csv file, see "User Defaults and Directories" on page 58.

3 For each subsequent line, enter a list of values separated by commas in the same order of column keywords listed in the first line.

Example:

```
login,name,home,itype,email,profile
```

```
myuser1,My User 1,/home/myuser1,Spectroscopy,
user1mai@abc.com,BasicLiquids
```

```
myuser2,My User 2,/home/myuser2,Spectroscopy,
user2mai@abc.com,CommonLiquids
```

To create multiple new user accounts from a .csv file

1 From the menu bar, go to **Management > Users**.

2 Select **New User**.

3 Select **Multiple Users** from the drop-down menu.

4 Select **New Users (2 or more)**.

5 Select the **Use File for User list input** check box.

6 Select the **Create** button.

7 Enter the file path for the .csv input file.

8 Select the **Add Users** button.

To delete multiple users through inputting a .csv file:

The input file format is technically the same as for adding users. The only required keyword and value are for "login". That means the file must have the word "login" in the first non-comment non-empty line.

1 From the menu bar, go to **Management > Users**.

2 Select **New User**.

3 Select **Multiple Users** from the drop-down menu.

4 Select **New Users (2 or more)**.

5 Select the **Use File for User list input** check box.

6 Select the **Delete** button.

7 Enter the file path for the .csv input file.

8 Select the **Delete Users** button.

Deleting a user account

Use this procedure to delete a user account.

1 Select **Management**.

2 Select **Users**.

3 Select **Show all VJ Users**.

4 Right-click the user's account and select **Delete**.

Only the user account is deleted-operators assigned to the account are not deleted. Operators can be assigned to other user accounts, see "Adding Operators to a User Account" on page 64, or deleted, see "Deleting Operators from User Accounts" on page 81.

The home directory and VnmrJ 3.2 files can be restored from the trash can if the trash can has not been deleted.

Restoring a user account

A deleted user account can be restored if the trash can has not been emptied.

1 Double-click the **Trash Can** icon.

The Trash Can window appears.
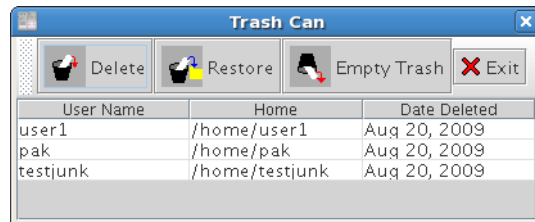
2 Select the account to be restored by clicking on it once.

3 Select **Restore**.

4 Exit the **Trash Can** window.

Converting user accounts to VnmrJ 3.2

Use this procedure to convert VNMR users to VnmrJ 3.2 users.

1 Select **Configure** from the VnmrJ 3.2 Admin interface.

2 Select **Users**.

3 Select **Convert users**.

The Change vnmr users to VnmrJ 3.2 users window appears. VNMR user accounts are listed on the left side of the screen.
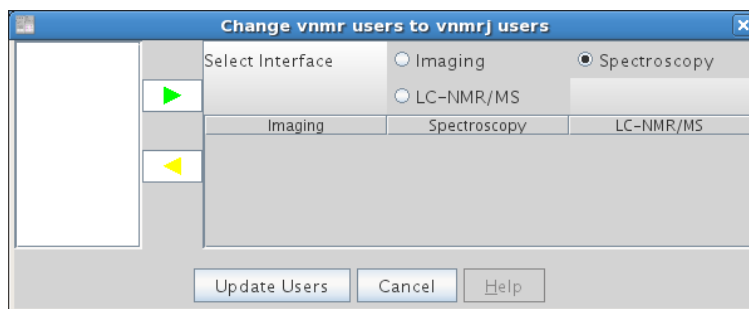
4 Click an **interface type** to sort by **interface type**.

5 Select the **VNMR account** to be converted.

6 Select the **interface type** and click the **green arrow**.

7 Hold the **Control** and **Shift** keys to make multiple selections of accounts with the same interface.

8 Repeat the previous step for other accounts using other interfaces.

9 Click **Update Users**.

Updating user accounts

Use this procedure to update multiple VnmrJ 3.2 user accounts.

CAUTION	Update user accounts after upgrading or reloading software.

1 Select **Configure**.
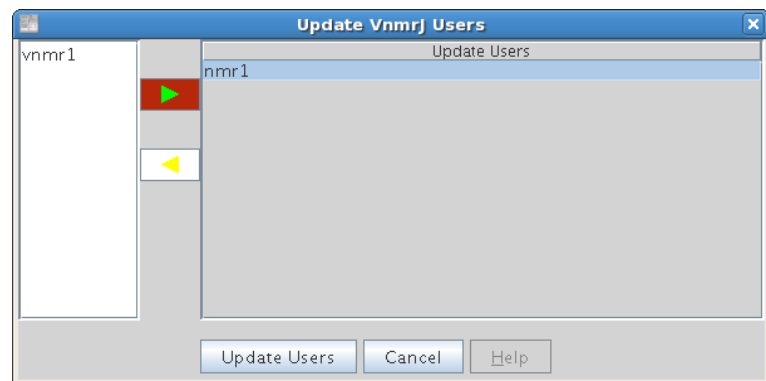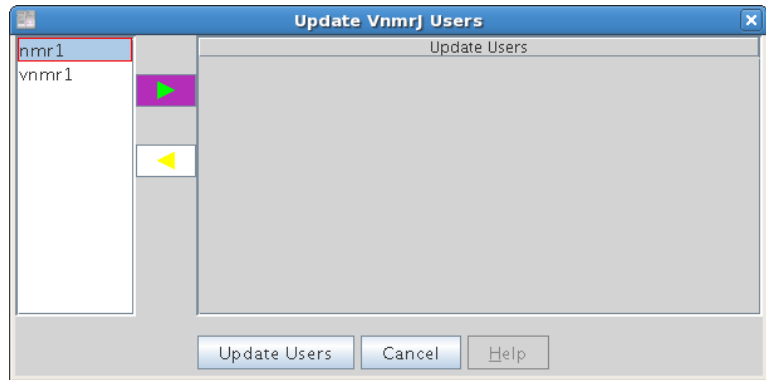
2 Select **Users**.

3 Select **Update Users**.

  The Update VnmrJ 3.2 Users window appears with VnmrJ 3.2 user accounts listed on the left side of the window.

4 Click an **interface** to sort by that interface.

5 Select the accounts to be updated.

6 Hold the **Control** and **Shift** keys to select multiple accounts with the same interface.

7 Click the highlighted, green arrow to move the accounts to Update Users.

8 Click **Update Users**.

User Defaults and Directories

Use the VnmrJ 3.2 Admin interface to set up user account defaults, templates, and directories.

User account defaults

Review and configure user account default properties before creating a new user account. These properties apply to all new VnmrJ 3.2 user accounts.

1 Select **Configure**.

2 Select **Users**.

3 Select **Defaults**.

The Defaults window appears and shows the defaults that will be used when a new user account is established.
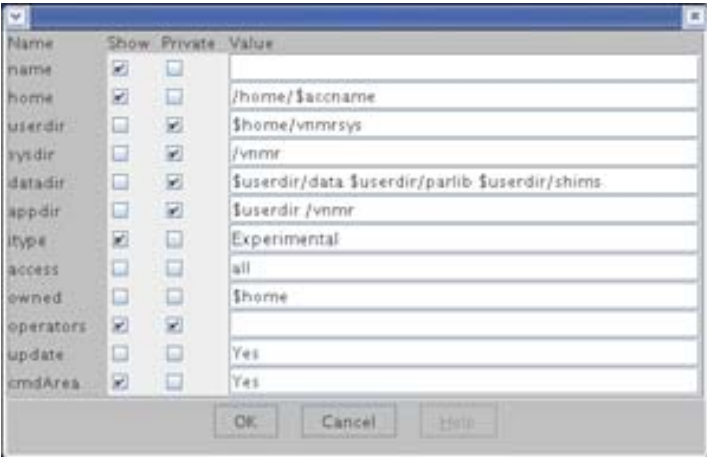
Field	Description
Name	Full name of a user.
Home	Home directory of a user.

Field	Description
Userdir	Directory that contains private VnmrJ 3.2 files for a user.
Sysdir	System directory for VnmrJ 3.2.
Datadir	Path of the directories where user data is stored.
Appdir	Directory search path used to search for application-specific files.
Itype	The itype field specifies the user interface. Spectroscopy for automation and manual operation systems.
Access	User's access level to other users' data
Owned	Directories that are owned by the user
Operators	Authorized account users. A system login is not required.
Update	When creating users, makeuser is automatically run to update user preferences if the value is set to Yes. This setting is only for operating system or VnmrJ 3.2 users who are already in the system
cmdArea	Show or do not show a command line.

4 Review the home field, which shows the path of a new user's home directory.

The default is set to /home/$accname.

The account name is $accname and /home is where the home directory of a new user account is located. This path is only used if the user is not a defined operating system user. The current home directory of existing operating system user is used.

Replace /home with the directory path to the user's home directory if /home does not exist or if the home directory of the user is located in another directory.

5 Review the itype field (the default interface type) for new VnmrJ 3.2 users.

6 Click **OK** to save your changes or **Cancel** to leave the settings unchanged.

User Directories and Data Saving Templates

User Directories and Data Saving Templates are now set up in the user preferences interface.

Console Display Sharing

Use this procedure to share the console display with the virtual network connection (VNC) viewers.

To enable:

1 From the VnmrJ 3.2 admin interface, click **Management**.

2 Click **Console Display Sharing...**

The Console Display Sharing window will appear.
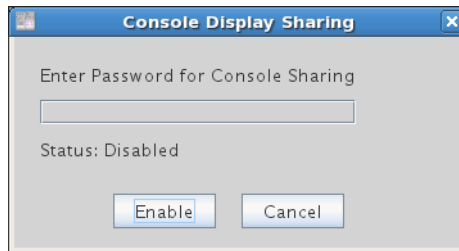
The status field shows if sharing is enabled or disabled. If disabled, a password entry box is present. This is the password one will use to remotely access and view the shared display (display 0).

3 Enter a password and click **Enable**.
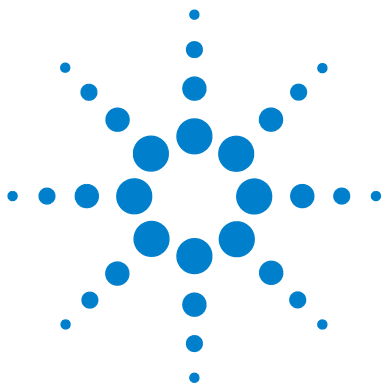
The window will now update. If this is the first time display sharing is turned on, the workstation needs to be rebooted.

To access the shared display, a new vnc viewer is needed, which will require the IP address of the workstation, the display (display 0) and the password provided in step 3.

To disable:

1 To disable Display Sharing, click the **Disable** button.

4

VnmrJ Account Administration

VnmrJ 3.2 administrative functions are controlled at the
VnmrJ 3.2 Admin level. Additional Spectroscopy
administration functions are controlled by the Spectroscopy
account owner. See Preferences in the *Automation User
Guide*.

Agilent Technologies

63

Adding Operators to a User Account

VnmrJ 3.2 operators can be added to user accounts. Operators are typically added to a Spectroscopy account owner- a Spectroscopy account with an operating system login. Typically, a Spectroscopy account owner sets up an automation run for operators to use. Operators can be VnmrJ 3.2- only operators or established VnmrJ 3.2 users.

1 Click **Show all VJ Users** and select the user account to which operated are to be added.

2 Enter the name of each operator, who has NMR privileges in the selected account in the VnmrJ 3.2 Operator field on the right panel.

Separate each operator with a space. The operators can have a mixture of VnmrJ 3.2 only operators and operators with both an operating system and VnmrJ 3.2 account.

Operators with no operating system account are assigned the default password, see "Setting Operator Default Password" on page 73.

Operators that have an operating system account use their operating system account password to access the VnmrJ 3.2 operator interface

3 Click **Save User**.

Creating Profiles - Spectroscopy Accounts

Implementing profiles

Implement the operator profile for the Spectroscopy account owner and operator. The system administrator creates and assigns a profile containing the protocols, rights, and tools that are available to a specific operator or assigned to several operators.

Protocols are selected from the available list of protocols or from the Profile pop-up, see Figure 6.
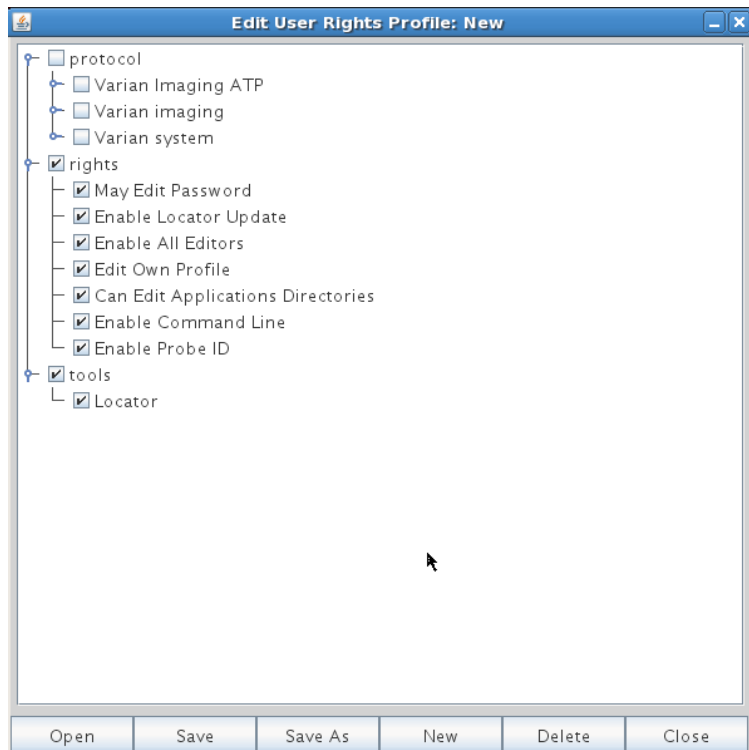
Figure 6   Edit user rights profile window

Rights are selected from the available rights listed in Table 14.

Table 14   User rights

Right	Function or action allowed
May edit password	Shows the Edit Password item in the Tools menu.
Enable locator update	Shows the following items in the Tools menu: Update locator submenu, Import files to locator, Save/Delete custom locator statement.
Enable all editors	Shows all items in the Edit menu, and show the Create protocols submenu in the Tools menu.
Edit own profile	Shows the Edit Config Profile item in the Edit menu.
Can edit applications directories	Allows applications edits.
Enable command line	Shows the Command Line.
Enable probe ID	Shows the Probe ID.

Table 15   User tools

Tools	Description
Locator	Accesses database search interface.

Table 16   User profiles

User profile	Description
AllLiquids	Contains all liquid protocols, all rights, and available tools.
BasicLiquids	Contains only a few protocols, a few rights, and available tools.
CommonLiquids	Contains common liquid protocols.

Table 16   User profiles (continued)

User profile	Description
BasicLiquidsSecure	Contains a few protocols, a few rights, and available tools.
AllImaging	Contains imaging protocols, all rights, and all tools.
AllSolids	Contains all solids protocols, all rights, and all tools.

Creating, Editing, Viewing, and Deleting Profiles

1 Start **VnmrJ 3.2 Admin**.
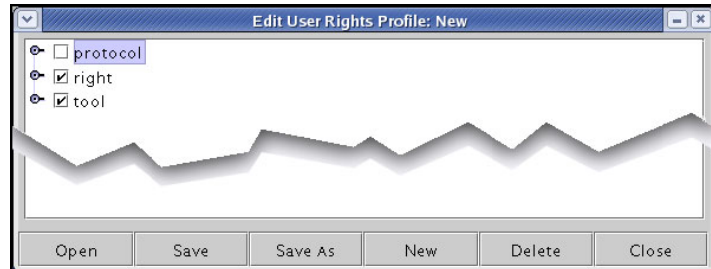
2 Click **Configure** in the main menu.

3 Select **Edit Profile**.

The Edit User Rights Profile window opens and displays the Profile named at the top of the window.

Creating a new profile

1 Select **New** to create a new profile.

2 Use the file tree controls to expand or contract the file tree:

- Expand — click the ● to change it to 🔻 .
- Collapse — click the 🔻 to change it to ● .

3 Set Rights as follows:

- Allow: Select the check box.
- Not Allow: Clear the check box.

4 Use the controls at the bottom of the **Edit User Profile** window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the Edit User Profile window.

Editing or viewing an existing profile

1 Select **Open** to edit an existing user rights profile.

2 Use the file tree controls to expand or contract the file tree:

- Expand — click the ⚬ to change it to ▽ .
- Collapse — click the ▽ to change it to ⚬ .

3 Do one of the following:

- Close after viewing the profile - Go to Step 5 and click **Close**.
- Continue and edit the profile by going to next step (Set Rights).

4 Set Rights as follows:

- Allow: Select the check box.
- Not Allow: Clear the check box.

5 Use the controls at the bottom of the **Edit User Profile** window to **Save** (uses existing file name), **Save As** (prompts for new file name), or **Close** (no change) the Edit User Profile window.

Deleting an existing profile

1 Click the **Delete** button to bring up a profile browser.

2 Select the user profile to be deleted.

3 Click the **Delete** button to delete or click the **Cancel** button to exit without deleting any profiles.

Assigning Operator Profiles

Assign a named profile to an operator using the VnmrJ 3.2 Admin interface as follows:

1 Start **VnmrJ 3.2 Admin**.

2 Click **Configure** on the main menu.

3 Select **Operators**.
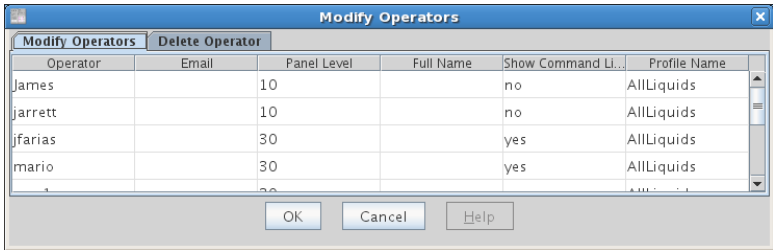
4 Select **Edit Operators...** to open the Modify Operators window. The last column in the Modify Operators window is for assigning the operator or account owner a Profile Name. The default is AllLiquids.

5 Click in the field under Profile Name for an operator to access the drop-down menu of profiles.

6 Select a **Profile** for operator rights. For custom profiles, see "Creating, Editing, Viewing, and Deleting Profiles" on page 68.

7 Click **OK** to apply the selected profile.

Setting Rights to Edit Applications Directories Search Paths

The user AllLiquids, BasicLiquids, and AllSolids profiles supplied with VnmrJ 3.2 set many rights including the Can Edit Applications Directories right. AllLiquids user profile enables the Can Edit Applications Directories right and the BasicLiquids user profile disables the Can Edit Applications Directories right. The AllSolids profile replaces the liquids experiments in the experiment panel with the full set of solids related experiments.

1 Start **VnmrJ 3.2 Admin**.

2 Click **Configure** in the main menu.

3 Select **Edit Profile**.
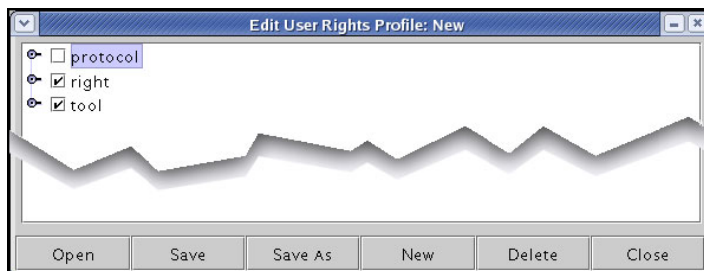
4 Expand the list under right by clicking on the ☞ to change it to ☞' .

5 Do one of the following:

• Select the check box next to Can Edit Applications Directories right, to allow the operator to edit the applications directory (default for experimental and walkup account owners).

1 Clear the box next to **Can Edit Applications Directories** right, to remove the right to edit the applications directory.

• Account login users with write permission to the `/vnmr/adm/users` directory and subfiles can set applications directories for all users. Account login users without these systems write permissions and having the **Can Edit Applications Directories** right can edit and customize their private applications directories. Account login users operators who are not granted the canEditAppdi right cannot change their applications directories.

2 Save the profile with new name or overwrite the current profile. Assign the profile to the operators associated with the spectroscopy account.

   1 Click **Configure**.

   2 Select **Operators**.

   3 Select **Edit operators...**

   4 Click in the **Profile Name** field for the operator.

   5 Select a Profile from the drop-down menu list. Continue for each operator.

   6 Click **OK** to set the assignments of the profiles and close the Modify Operators window.

3 Click **Save User**.

4 Click **Management**.

5 Click **Exit** to close the VnmrJ 3.2 Admin window.

Setting Operator Default Password

Set the default password for VnmrJ 3.2 operators who do not have an operating system login:

1 Select **Configure**.

2 Select **Operators**.

3 Select **Preferences**.

The Preferences window appears.

4 Enter a default password in the password field for operators who do not have an operating system login.

Operators with an operating system account login use the operating system account password to access the walkup operator interface. Operators, both with and without an operating system account, can change their passwords by selecting Change Password from the Tools menu on their interface. Change Password will change both the Operator and operating system login password, if an operating system account exists.

5 Click **OK**.

Resetting Operator Password

This applies only to operators that do not have an operating system (OS) account login. Refer to the OS manual(s) to reset the password for an operator/OS account.

Reset an operator's password to the default password set in, "Setting Operator Default Password" on page 73, by entering the operator name and clicking on OK.

Modifying Operators

Opening the modify operators window

1 Start the **VnmrJ 3.2 Admin** interface.

2 Select **Configure**.

3 Select **Operators**.

4 Select **Edit** operators.

The Modify Operators window appears.
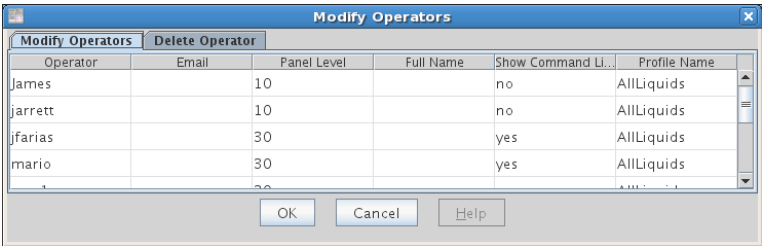
5 Select the **Modify Operators** tab.

Adding or editing operator's email

If the operator's email is added, the operator is notified when a sample is finished.

1 See "Opening the modify operators window".

2 Edit or add an e-mail address.

3 Do one of the following:

- Continue with "Setting Panel Levels and Command Line Access".

- Click **OK** to close the Modify Operators window.

- Click **Cancel** to exit from the Modify Operators window and make no changes.

Setting Panel Levels and Command Line Access

Panel levels are set by the VnmrJ 3.2 Administrator and determine which VnmrJ 3.2 interface pages are available under the tabs in the parameter page area. Setting panel levels applies only to walkup account owners and walkup account operators. The default is 10 for operators and 30 for the account owner. Setting the panel level higher allows for more pages to be available. The experimental VnmrJ 3.2 account has a fixed panel level of 100.

NOTE	Panel levels can only be changed during the operator login process in the Walkup interface.

1 See "Opening the modify operators window" on page 75.

2 Change the panel level for any operator by entering a value in the Panel Level cell for the operator.
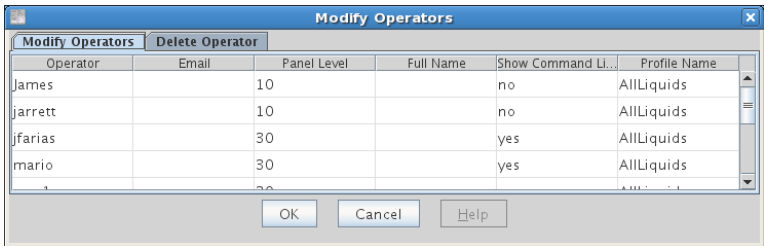
Panel level values and displayed pages are:

Value	Display
0-9	Shows minimum number of pages.
10-29	No shim, lock, or processing, and minimal parameter control is available. This may be used for routine automation users and is typical for a basic user.
	Shim and lock are available only if there is a no sample changer. Basic processing is available. Pages are not fully populated, allowing control of a few basic parameters.
30-49	All pages are available and fully populated.

3 Type Yes in the field under Show Command Line to give each operator command line access. The default is no command line access.

4 Do one of the following:

- Continue to the next section.
- Click **OK** to close the Modify Operators window.
- Click **Cancel** to exit the Modify Operators window and make no changes.

Adding operators full name
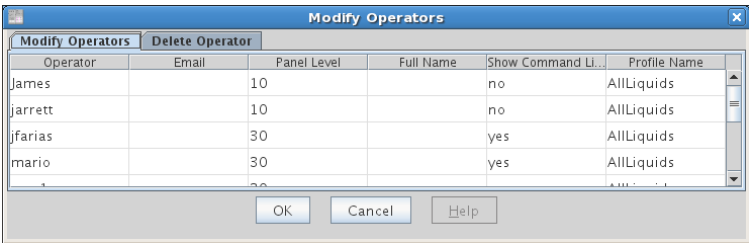
1 Edit or add the full name of the operator in the field below Full Name.

2 Do one of the following:

- Continue with "Viewing command line access".

- Click **OK** to close the Modify Operators window.

- Click **Cancel** to exit the Modify Operators window and make no changes.

Viewing command line access

1 See "Opening the modify operators window" on page 75.

The command line access is displayed in the field below Show Command Line in the operator's row.
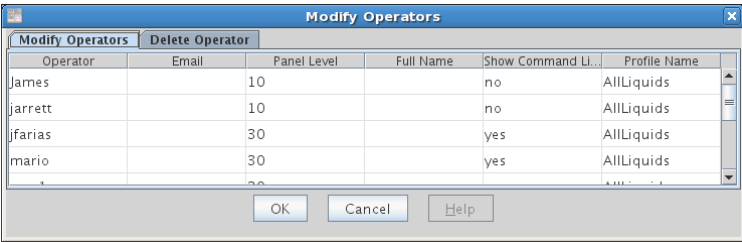
2 Access to the command line is set by "Setting Panel Levels and Command Line Access" on page 77 or by "Adding or editing user profiles".

3 Do one of the following:

- Continue with "Adding or editing user profiles".
- Click **OK** to close the Modify Operators window.
- Click **Cancel** to exit the Modify Operators window and make no changes.

Adding or editing user profiles

1 See "Creating Profiles - Spectroscopy Accounts" on page 65.

2 Create or edit an existing user profile.

3 Close the Edit User Rights Profile window.

4 Write down the name or names of the user profiles that will be assigned to the operators.

5 See "Opening the modify operators window" on page 75.

6 Type the name of the profile (with no extension) in the field below Profile in the operator's row.

Operator	Email	Panel Level	Full Name	Show Command Li...	Profile Name
James		10		no	AllLiquids
jarrett		10		no	AllLiquids
jfarias		30		yes	AllLiquids
mario		30		yes	AllLiquids
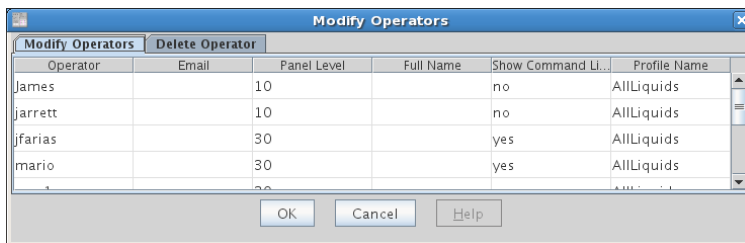
7 Do one of the following:

- Click **OK** to close the Modify Operators window.
- Click **Cancel** to exit the Modify Operators window and make no changes.

Deleting Operators from User Accounts

Operators can be removed from all accounts or from a single account.

Deleting operators from all assigned accounts

1 Select **Configure**.

2 Select **Operators**.

3 Select **Delete Operator**.

The **Modify Operators** window appears displaying the Delete Operators tab.

4 Select the operators to be removed and click **OK**.

Deleting an operator from a single account

1 Select a user account.

The operators are listed in the right panel, in the VnmrJ 3.2 Operators field.

2 Delete the operator(s) from the list.

3 Click **Save User**.
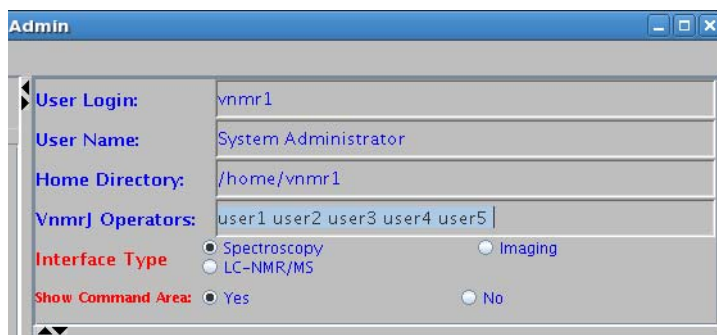
Changing the Icon on the Operator Login Screen
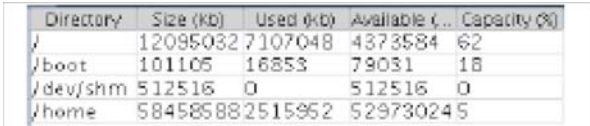
The Default Operator Login window contains the Agilent Technologies, Inc. logo, which is a GIF file. Change the logo as follows.

1 Select **Configure**.

2 Select **Operators**.

3 Select **Preferences** to display the Preferences window.

4 Enter the complete path to the GIF file.

5 Click **OK**.

Viewing the File System

The lower right panel of the VnmrJ 3.2 Admin interface shows information about the operating system.

The Select Directory tab has the following icons:

Instruction/button/icon	Description or window
1 Select **UNIX**. **2** Select **File System**. The View Directories window opens.	
Disk space window	
Disk space window displays information about mounted network directories, disk partitions, size, space used, space available, available capacity. This same information is also shown from Disk Space tab in the VnmrJ 3.2 Admin Interface.	
	Change the directory to selected directory.
	Go to admin's */home* directory.
	Create a new directory in the current directory.
	List files with small icons.
	List files with small icons and details.
Look In drop-down menu	Select a directory from the drop-down list. Click a directory in the directories window to select a directory. The directory is inserted in the empty directory field of user directories. See "User Directories and Data Saving Templates" on page 60.

5
Configuring Printers for VnmrJ 3.2

Use the Linux Printer Set window, wizard, and Vnmr Plotter Configuration window to add or manage a printer.

NOTE	Adding or managing a printer is done by the Linux or VnmrJ 3.2 administrator.
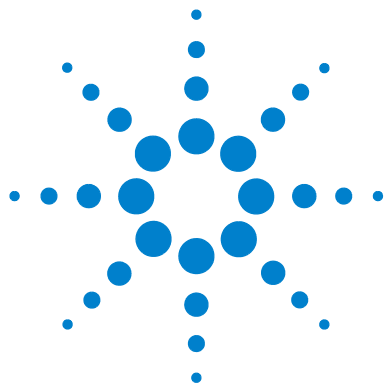
Setting Up a Linux Printer

As the Linux or VnmrJ 3.2 administrator, use this procedure to set up a printer.
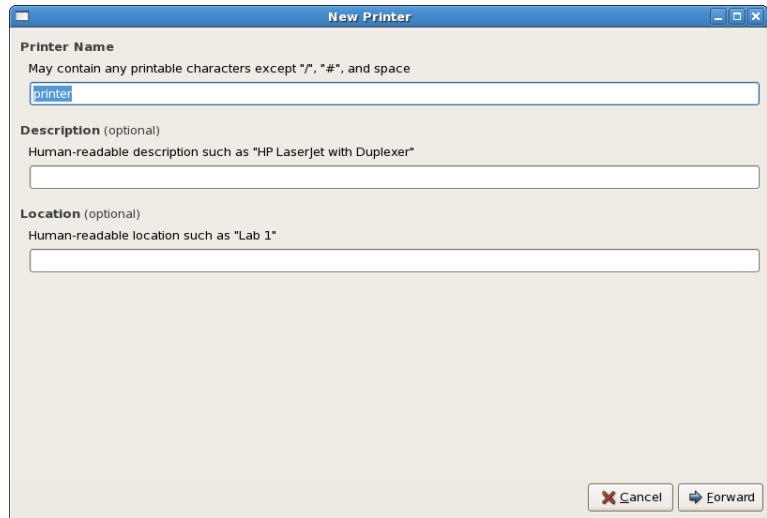
1 Click the Linux **System** menu.

2 Select **Administration**.

3 Select **Printing**.

4 Enter the root user's password in the pop-up window.

The Printer Configuration window appears. Use this window to configure, add, or remove Linux printers.

5 Click **Print Test Page** to verify proper printer configuration.
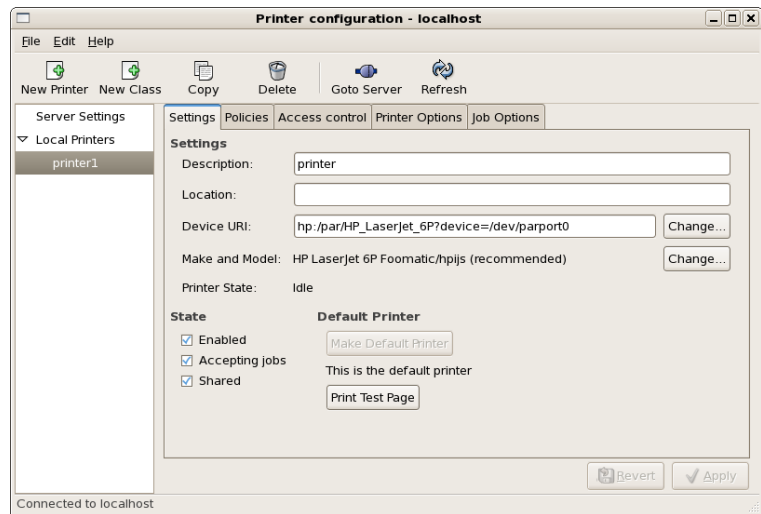
6 To add a new printer, click **New Printer**.
A New Printer wizard is displayed to assist in adding a printer.

7 Enter a `Printer Name`, `Description`, `Location`, and click **Forward**.

8 Select the printer connection then click **Forward**.
The wizard detects and lists printers that are turned on
and connected to the workstation.
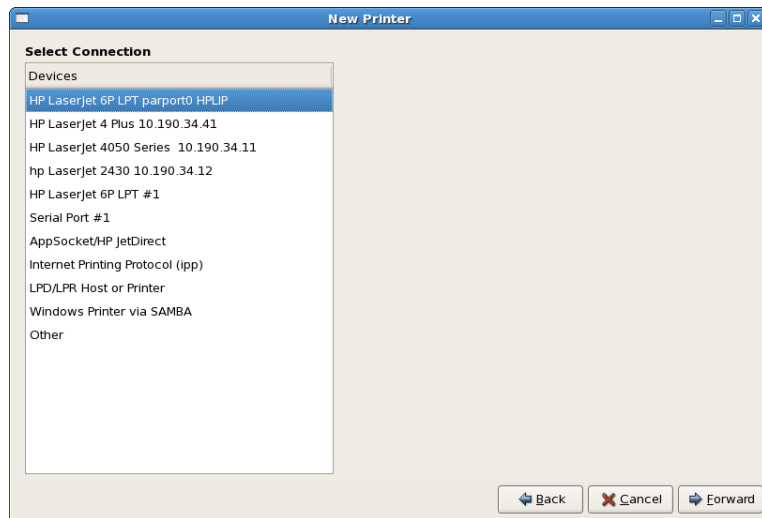
9 Select a PostScript Printer Description. Then click **Forward**.

10 Select the printer. The wizard highlights the detected printer.
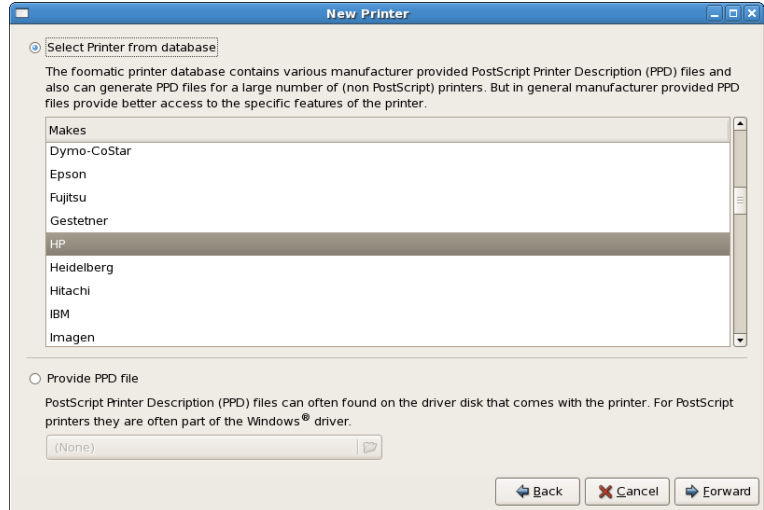
11 Select the printer model and driver, and then click **Forward**.

The wizard highlights the detected printer's model and default driver.
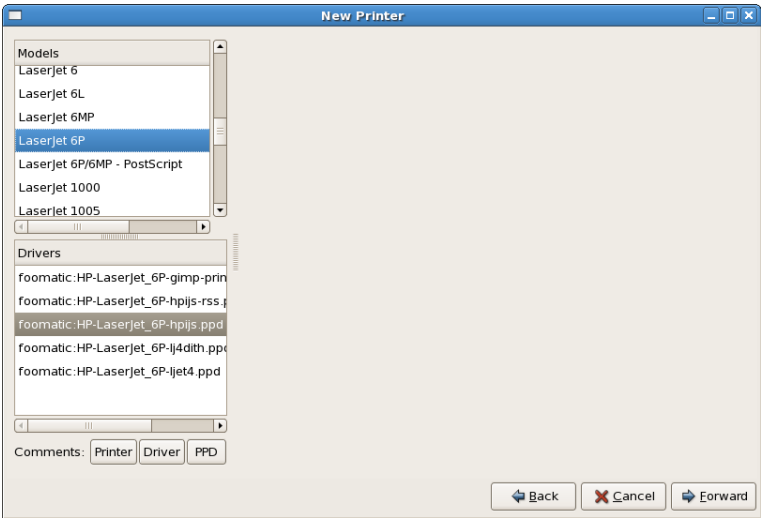
12 Click **Apply** to create the new printer.
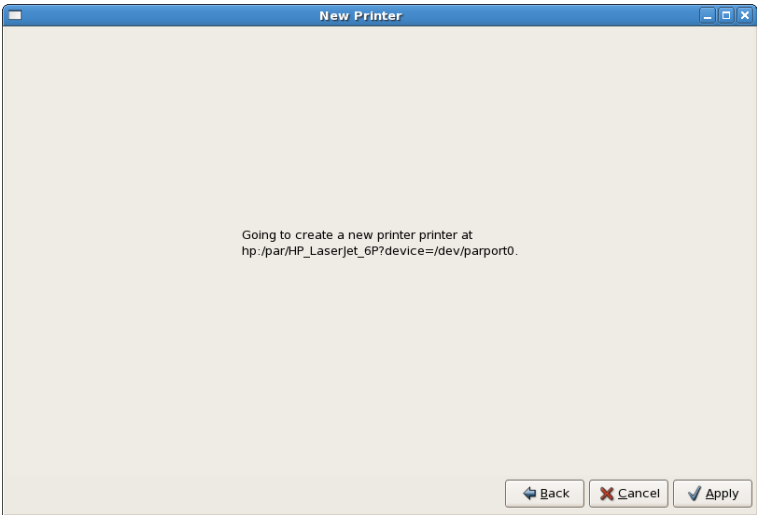
13 Print a test page from the **Printer Configuration** window to verify proper configuration of the printer.

NOTE	To delete a printer, select the printer in the Printer Configuration window and click the Trash Can icon.

Setting up a Windows Printer for VnmrJ 3.2

The following procedure is for Windows 7 OS. Procedures for Windows XP may differ slightly.

1 Go to Start > Devices & Printer.

2 On the Devices & Printer window, right-click on the desired printer and click **Properties**.

3 Select the Sharing tab and click **Change Sharing Options**.
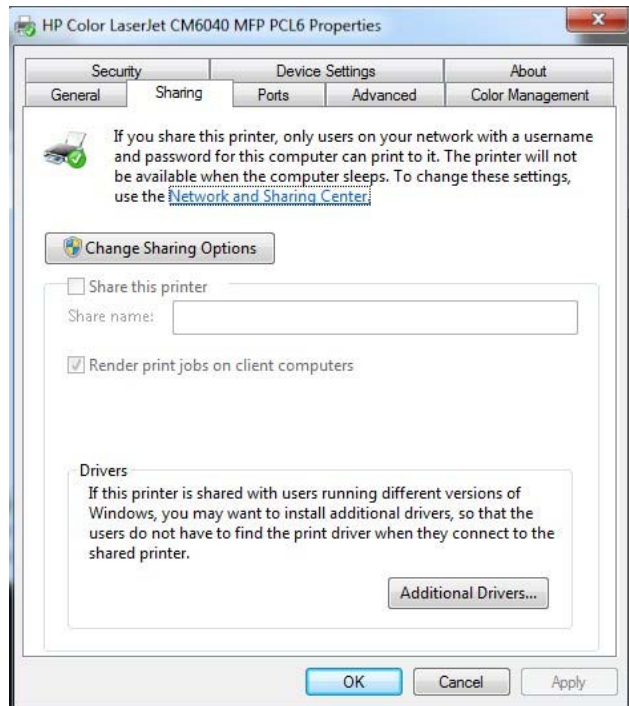
4 Select **Share this printer** and enter the share name without spaces.

5 Click **Apply**, then **OK**.
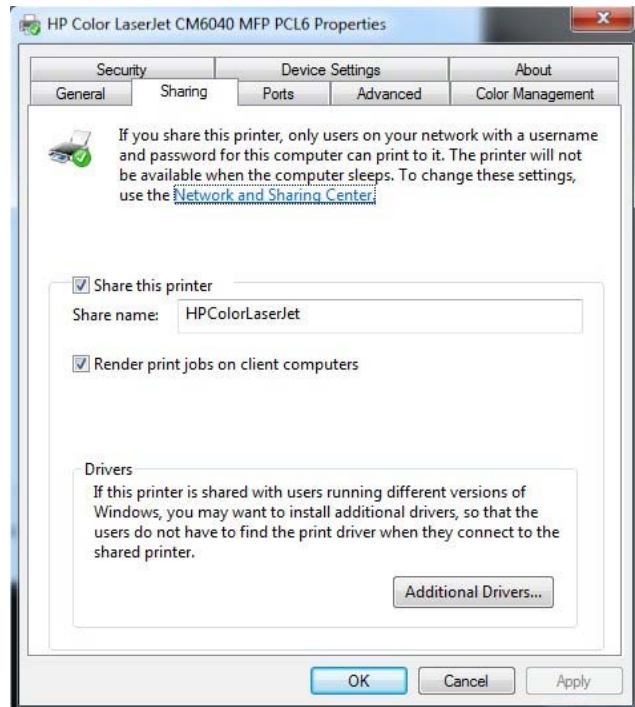
Setting Up a Printer for VnmrJ 3.2

Set up a VnmrJ 3.2 printer using the VNMR Plotter Configuration window.

1 Click the **VnmrJ 3.2 Admin** icon.

2 Click **Management**.

3 Select **Printers...** to open the VNMR Plotter Configuration window.
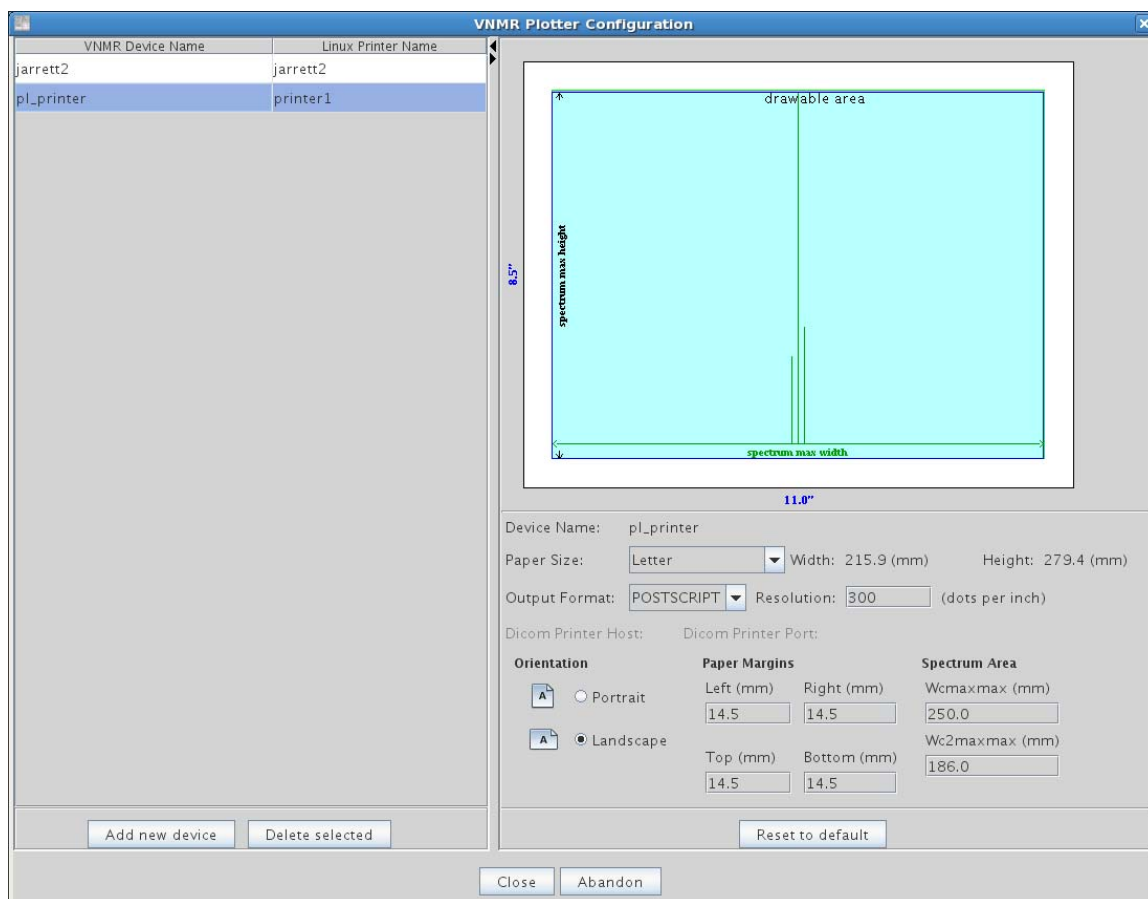
4 Select an available printer from the Linux Printer Name pull-down menu.

5 Enter in a Name that VnmrJ 3.2 will use to recognize this printer in the VNMR Device Name entry window.

6 Configure VnmrJ 3.2 page settings on the right of the VNMR Plotter Configuration window: paper size, output format, dots per inch (dpi), paper orientation, and printable area.

NOTE	The **Reset to default** button resets the printer configuration to the last saved settings. It does not restore the settings to a "factory default."

7 Click **Close** to save and close the VNMR Plotter Configuration. To abandon all changes, click **Abandon**.

8 To delete a printer, select the printer in the VNMR Device Name column.

9 Click **Delete selected**, then click **Close** to save the deletion and close the VnmrJ 3.2 Plotter Configuration window.

NOTE	To use a non-standard device type, create a printer with the VNMR Plotter Configuration window then edit that printer entry in the */vnmr/devicenames* file to contain the appropriate type. See Table 17 for various types and descriptions.

Table 17   VnmrJ 3.2 printer and plotter types with descriptions

VnmrJ 3.2 device type	Description
HP7475A	HP7475 plotter
HP7550A	HP7550 plotter using 11x17 inch paper
HP7550A8	HP7550 plotter using 8 1/2 x 11 inch paper
DeskJet_300	HP DeskJet using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
DeskJet_300R	HP DeskJet using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
DraftPro_C	HP DraftPro plotter using size C paper

Table 17   VnmrJ 3.2 printer and plotter types with descriptions (continued)

VnmrJ 3.2 device type	Description
DraftPro_D	HP DraftPro plotter using size D paper
DraftMaster_A	HP DraftMaster plotter using size A paper
DraftMaster_B	HP DraftMaster plotter using size B paper
DraftMaster_C	HP DraftMaster plotter using size C paper
DraftMaster_D	HP DraftMaster plotter using size D paper
DraftMaster_E	HP DraftMaster plotter using size E paper
LaserJet_150	HP LaserJet (or DeskJet) using 150 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
LaserJet_150R	HP LaserJet (or DeskJet) using 150 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_300	HP LaserJet (or DeskJet) using 300 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
LaserJet_300R	HP LaserJet (or DeskJet) using 300 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_B_300R	HP LaserJet (or DeskJet) using 300 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_300R	HP LaserJet (or DeskJet) using 300 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LaserJet_4550	HP Color LaserJet using 600 dpi.
LaserJet_600R	HP LaserJet (or DeskJet) using 600 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_B_600R	HP LaserJet (or DeskJet) using 600 dpi, B-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
LJ_A3_600R	HP LaserJet (or DeskJet) using 600 dpi, A3-size paper, and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS_A	PostScript printer using vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value is not recommended.

Table 17   VnmrJ 3.2 printer and plotter types with descriptions (continued)

VnmrJ 3.2 device type	Description
PS_AR	PostScript printer (for example, PS4069) using horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
PS4079_HPGL	Lexmark PS4079 or PS4079 plus using 11x17 inch paper in HPGL mode. HPGL mode is required for color output.
QuietJet_96	HP QuietJet using low 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_96R	HP QuietJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
QuietJet_192	HP QuietJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
QuietJet_192R	HP QuietJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_96	HP ThinkJet using 96 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_96R	HP ThinkJet using 96 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.
ThinkJet_192	HP ThinkJet using 192 dpi and a vertical (portrait) orientation in which only the top part of the page can be used for plotting. This value not recommended.
ThinkJet_192R	HP ThinkJet using 192 dpi and a horizontal (landscape) orientation in which the entire page can be used for plotting, and a vertical orientation for printing.

6

Automated Hardware

This section describes how to configure software to control
automated hardware. Set up procedures require system
hardware administration access, typically vnmr1, and may
require VnmrJ 3.2 system administrator access.

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Setting Up Automated Sample Handling

1 Log in as the system hardware administrator.

2 Click **Edit** on the main menu.

3 Select **System settings**.

4 Click the **System config** button.

5 Click the **drop-down** menu next to the Sample Changer field and select a sample changer option.
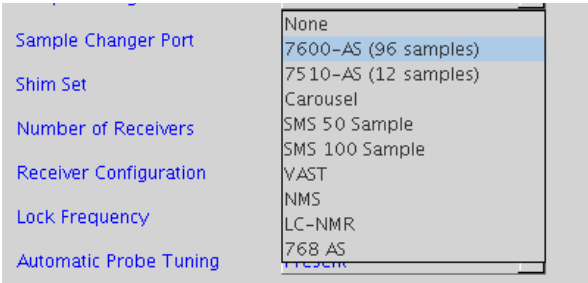
6 Click the **drop-down** menu next to the Sample Changer Port field.

7 Select a sample changer port.

8 Click the **drop-down** menu next to the Sample Changer Port field.

SMS 50, 100, NMS, Carousel, VAST, LC-NMR	Select Com1
7600-AS, 7510-AS, 768AS	Select Ethernet
Not used or no sample handler	None

Operating and other instructions specific to an automated sample handing option are contained in the Automation manual and their corresponding hardware manuals.

9 Click **OK**.

Setting Up Automatic Probe Tuning

Configuring the Software for ProTune

1 Log in as the system hardware administrator, typically vnmr1.

2 Click **Edit** on the main menu.

3 Select **System Settings**.

4 Click the **System config** button.

5 Select **Present** from the drop-down menu next to the Automatic Probe Tuning field.

6 Click **OK**.

7 Continue with "Loading chan# and motor# Persistence Files".

Loading chan# and motor# Persistence Files

AutoX and PZT compatible probes ship with a CD containing Persistence files (chan# and motor# files) specific to that probe. These files characterize the probe for the Automatic probe tuning accessory and are used the first time the probe is automatically tuned.

Load the Persistence files as follows:

1 Insert the CD with probe Persistence files into the CD ROM drive.

2 Open a terminal window and do one of the following:

Locate the system **probe** file.

a Type:
```
cd /vnmr/probes
ls
```

b Write down the <name of probe file>.

c Continue with step 3.
Create a probe system file.

d Follow the procedure in "Setting up, selecting, and creating a probe calibration file" on page 142.

e Type:
```
cd /vnmr/probes
ls
```

f Verify and write down the <name of probe file>.

g Continue with step 3.

3 Type:

```
cd /vnmr/tune
mkdir <name of probe file>
```

4 Change to the CDROM directory and enter one of the following:

```
cd /media/cdrecorder
```

5 Copy the Persistence files from the CDROM to the created probe directory:

Type: `cp * /vnmr/tune/<name of probe file>`

6 Verify that the files were copied.

Type: `ls /vnmr/tune/<name of probe file>`

The new ProbeName directory should contain six chan# files (chan#0 through chan#5) and six motor# files (motor#0 through motor#5).

ProTune software copies the probe Persistence files to the directory *~user/vnmrsys/tune* the first time it is run by a user. If the directory has not been created, the directory is created. A database of reference values is maintained in the local directory.

Setting / Resetting the Phase for Automatic Probe Tuning

This section provides instructions for setting or resetting the phase for ProTune. It may be necessary to reset the phase if the NMR console has been power cycled.

Starting the ProTune GUI

1 Log in as the system hardware administrator, typically vnmr1.

2 Start the VnmrJ 3.2 by clicking on the **VnmrJ** icon.

From the command line, type `protune('calibrate')`. The ProTune GUI appears.
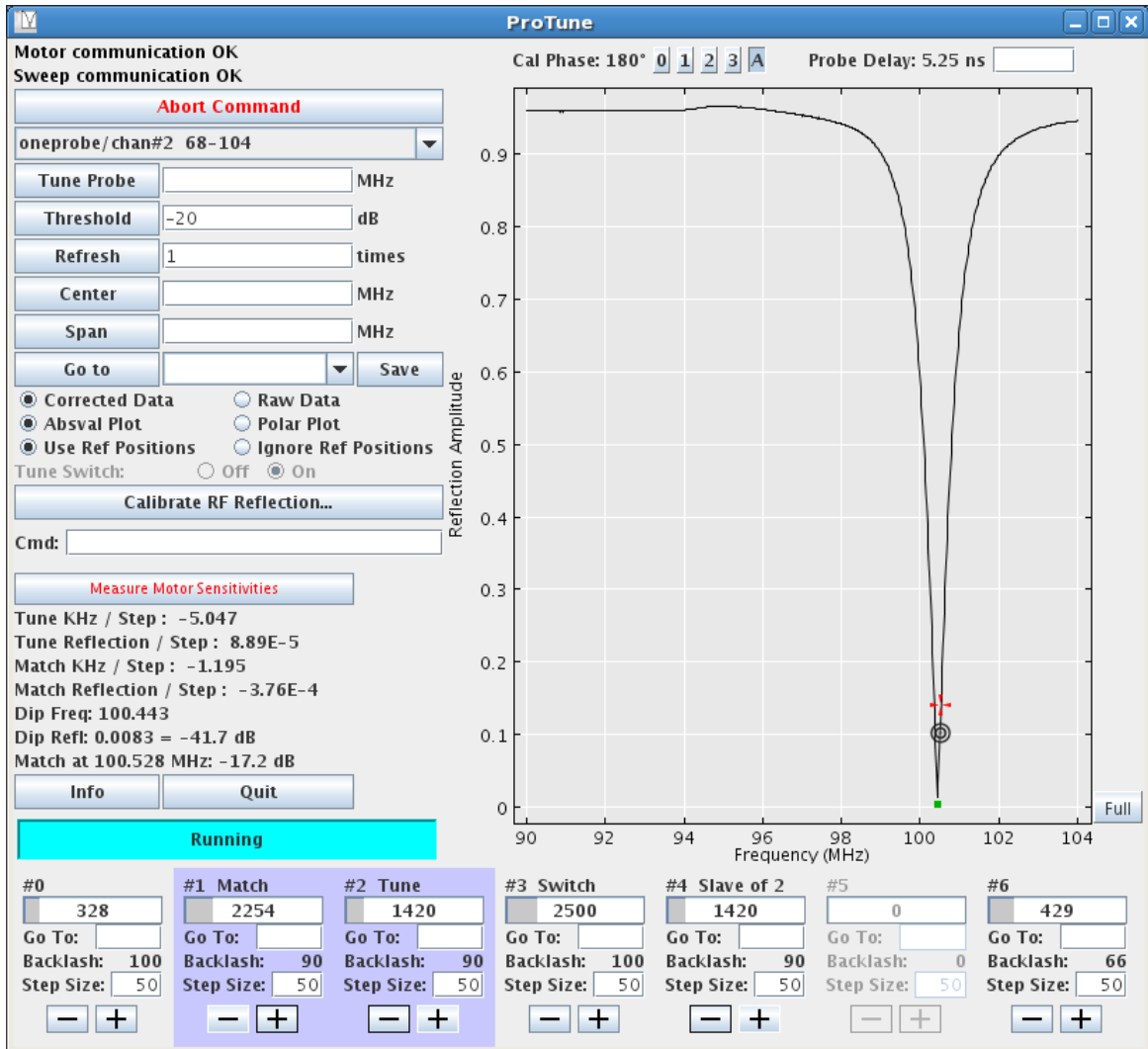
3 Click the **A** button located in the top center of the ProTune GUI for the program to automatically find the best phase.

NOTE   One can manually set the phase by clicking on the **0, 1, 2, 3** buttons and observing the displayed reflection. The phase which provides the flattest base is the phase to save.

6   Automated Hardware

7

VnmrJ 3.2 Accounting Administration

The VnmrJ 3.2 Accounting tool provides NMR administrators an effective way to keep a log of VnmrJ 3.2 users. Use VnmrJ 3.2 Accounting to create groups of console users with single-rate or multi-rate billing, show and print invoices and accounting reports.

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Starting VnmrJ 3.2 Accounting

Start VnmrJ 3.2 Accounting from:

- VnmrJ 3.2 Admin
  a Log in as the system administrator, typically vnmr1.
  b Start **VnmrJ 3.2 Admin**.
  c Click **Management** in the menu bar.
  d Select **Cost/Time Accounting**.
- Terminal Window
  a Open a terminal window.
  b Change users to the system administrator if the terminal window is not opened while logging in as the system administrator.
  c Type vnmr_accounting

VnmrJ 3.2 Accounting Window Interface

Billing

Click the **Billing** tab to open the Billing window. See Figure 7.
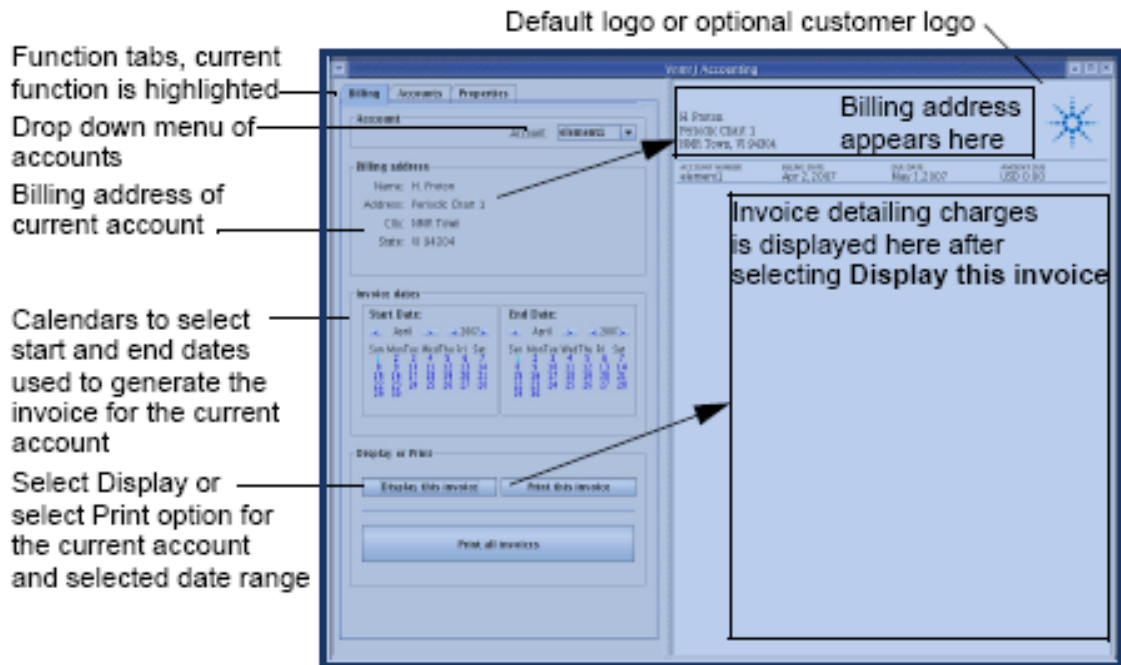
Figure 7   VnmrJ 3.2 accounting billing window

Accounts

Click the **Accounts** tab to open the Accounts window; see Figure 8.
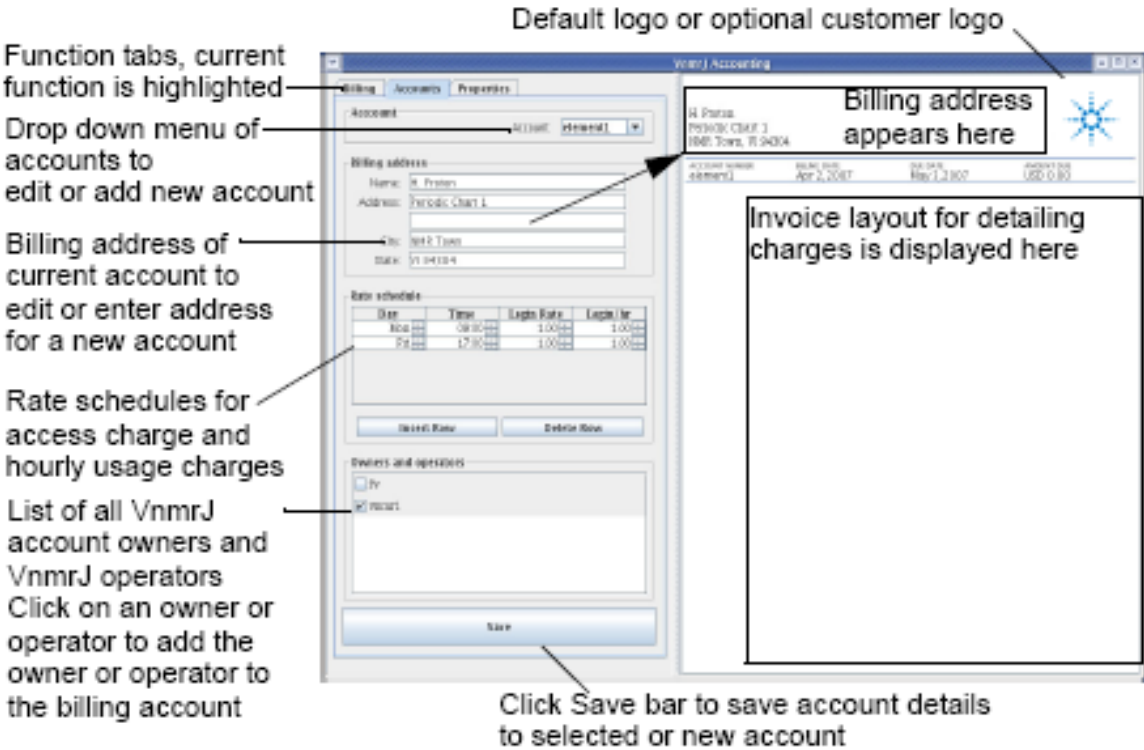
Figure 8   VnmrJ 3.2 accounting accounts window

Properties

Click the **Properties** tab to open the Properties window; see Figure 9.
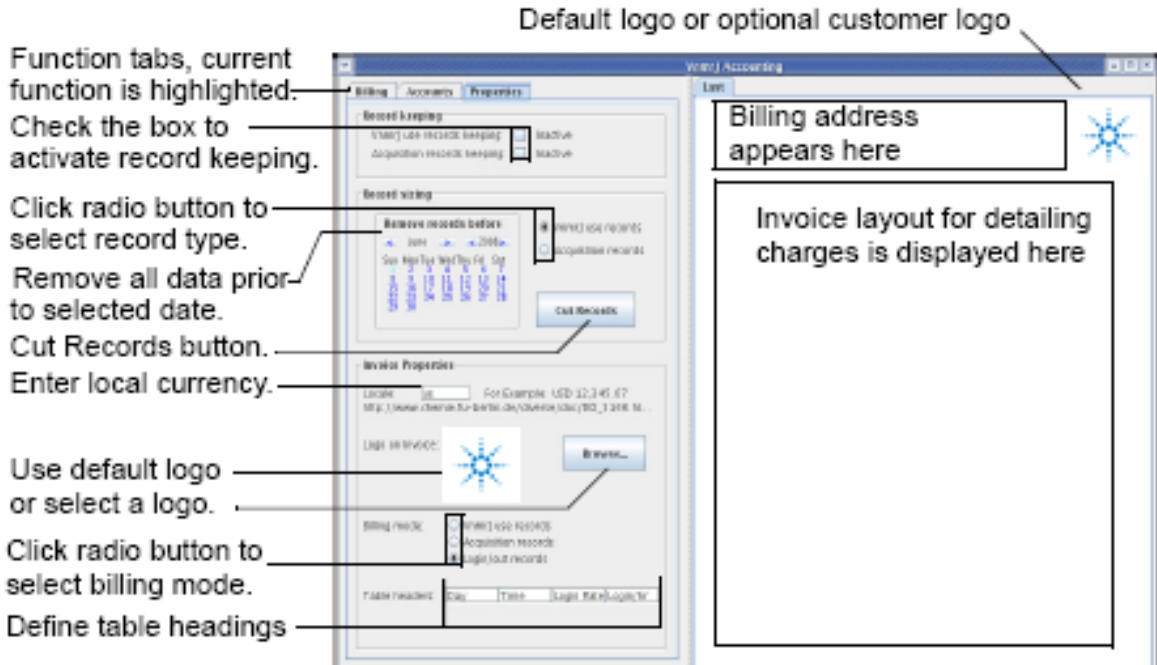
Figure 9   VnmrJ 3.2 accounting properties window

Generating Invoices

1 Start VnmrJ 3.2 Accounting if it is not running.

2 Select the **Billing** tab.

3 Select an account number from the drop-down list of accounts in the **Account:** field.

4 Select the start day using the **Start Date:** calendar controls as follows:

   a Select a month and year using the calendar controls.

   b Select a date by clicking on the calendar date in the selected month and year.

5 Select the end day using the End Date: calendar controls as in step 4.

6 Do one of the following:

Print Invoice for currently displayed account

   a Click the **Display this invoice** button to display the invoice on the right side of the Billing tab; see Figure 7 on page 109.

   b Click **Print this invoice** to print the displayed invoice.

Print invoices for all accounts on system

   a Click **Print all invoices** to generate an invoice for each account on the system.

   b Click **Print Summary** button to print out the summary page. The summary can be saved as a comma separated value (.csv) file for use with other software.

Creating or Editing an Account

A billing account gathers the time and use charges for system login account owners and any operators with privileges to use the system login account.

1 Create any required system login accounts that are required, see "User Account Administration" on page 49.

2 Add any required operators to each system login in account; see "Adding Operators to a User Account" on page 64.

3 Start **VnmrJ 3.2 Accounting**, see "Starting VnmrJ 3.2 Accounting" on page 108.

4 Select the **Accounts** tab.

5 Enter an account name in the **Account** field in the Account region or select an existing account number from the drop-down menu.

Account name can be alphanumeric, a combination, and can contain dashes or underlines. Do not use spaces, special characters, or non printing characters. Any string that is a legal filename may be used.

6 Complete the Billing address information work sheet for a new account or edit the information as required to update of an existing account.

7 Create or edit the billing rate, see "Establishing or Editing a Billing Rate Schedule" on page 115.
Add owners and operators whose usage is tracked and billed to this new account by selecting the checkbox next to the owner or operator.

8 Click **Save** to save the new or updated account information.

Establishing or Editing a Billing Rate Schedule

Billing rates

Usage is billed at the sum of the hourly rate times the number of hours plus the login or go rate charge.

The rate schedule for the current account is shown in the Rate schedule region. A new account will have only one billing row. An existing account will have one or more billing rows.

1 Enter account values for: Set the day, time, login rate, and hourly rate (Login billing default) or set the day, time, Go rate, Go hourly rate (Acquisition billing default) by using the control to set the required value or enter the information into the fields.

2 Insert or delete rows as required.

To insert a new row:

a Place the cursor in any field of the row below which a new row is required.

b Click the **Insert Row** button to add a row below the row with the cursor.

To delete a row:

a Place the cursor in any field of the row to be deleted.

b Click the **Delete Row** button to delete the row.

3 Click the **Save** button to save the new rate schedule for the current account.

Billing rates example

The billing period and rate begins on the day specified in the Day field at the time specified in the Time field and continues at the specified rate until a new time (on the same day) or new time and day are encountered. The rate of the last row applies until the time specified in the first row.

Set up a weekday/weekend schedule as follows:

1 Set the day on the first row to Mon.

2 Set the Time to 06:00 (6 AM). Change the hours using up and down arrows by double-clicking on the hours first. Change the minutes using up and down arrows by double-clicking on the minutes first. The time can also be entered.

3 Set a Rate for Login or Go.

4 Set the hourly rate.

5 Add a new row below the current row.

6 Set the day on the new row to Sat.

7 Set a new time of 00:01 (12:01 AM Saturday morning).

8 Set a new Rate.

9 Set a new hourly rate.

The weekday rate in this example begins at 06:00 hours on Monday and continues until one minute past midnight on Friday or 00:01 hours Saturday morning. The weekend rate continues until 06:00 hours Monday morning when the weekday rate starts.

Controlling Properties

Properties apply to all system accounts.

Enable/disable record keeping

1 Select the **Properties** tab to display the current account properties.

2 Activate the record keeping type by selecting the check box next to the type of record keeping:

- Login/out records keeping
- Acquisition records keeping

The label changes from inactive or on hold to active when the box is selected.

3 Type the command `su acqproc` twice if the Acquisition record keeping is (re)activated.

Reducing record size

The accounting record files can be large over time. To reduce their size:

1 Select a month and year using the calendar controls.

2 Select a date by clicking on the calendar date in the selected month and year.

3 Select **Logout records** or **Acquisition records**.

4 Click the **Cut Records** button.

Invoice Properties

Locale

Enter a two letter local code in the **Locale** field to establish the billing currency correct currency format. Local codes and currency formats are available at:
http://www.chemie.fu-berlin.de/diverse/doc/ISO_3166.html

Logo

Keep the default Agilent logo or select a custom logo using the **Browse** button. Place any custom logo in `/vnmr/adm/accounting/` as `.gif files`. The default logo is 87x70 pixels. The logo does not have a size limit and the invoice layout can adjust to accommodate logo size.

Billing modes

Account billing is determined by one of two billing modes: Acquisition Time, VnmrJ Use.

Acquisition Time

Tracks the time from start to completion and processing of an experiment. This is tracked in: `/vnmr/adm/accounting/gorecords.txt`

VnmrJ Use

Tracks the time the owner or operator starts or logs into VnmrJ 3. this implementation is used to track operator time during walkup, owner time in walkup or experimental mode, or both. If more than one VnmrJ 3.2 is opened, both are tracked and invoiced. This is tracked in: `/vnmr/adm/accounting/loginrecords.txt`. This is the only method to track operator time. This was previously referred to as Login or Logout Use.

File Locations

- Account information —

  ```
  /vnmr/adm/accounting/accounts/<account>.txt
  ```
- Records —

  ```
  /vnmr/adm/accounting/gorecords.txt
  /vnmr/adm/tmp/macrorecords.txt
  ```
- Logo —

  ```
  /vmnr/adm/accounting/*.gif
  ```
- Properties file —

  ```
  /vnmr/adm/accounting/accounts/accounting.prop
  ```

Properties File Contents

The `/vnmr/adm/accounting/accounts/accounting.prop` file contains the properties and keyword-value pairs required to customize the accounting software. Use the controls under the **Properties** tab to maintain this file. Each keyword-value pair appears on a separate line and is formatted as:

`keyword<space>=<space>value`

Lines starting with the # character are treated as a comment and ignored.

Currency

Enter the two-letter name for the country (for example, us for United States, de for Germany) to set the number format and currency symbol for the local. Refer to the following Website for a complete list:
http://www.chemie.fu-berlin.de/diverse/doc/ISO_3166.html.
The currency keyword defines currency symbol used in the invoice Amount Due and determines the use of the decimal period or comma in numbers.

Billing mode

Invoices are written based on the billing mode; Login time or Acquisition time, the choices are mutually exclusive.

`billingmode = macros`

Time is tracked by the `operatorlogin` and `operatorlogout` macros. When the file `/vnmr/adm/accounting/macrorecords` exists, these macros will record one line for each login and logout. The file is in ASCII and has world read/write permissions.

`billingmode = goes`

Time is tracked for any `su`, `go`, `ga`, `au`, `shim`, `lock`, `spin`, `change`, or `sample` command. One data line is written for each acquisition when the file `/vnmr/adm/accounting/gorecords.xml` exists and the following are recorded:

- account — usually ""
- operator — the operator name
- goflag — whether su, go, au, etc.
- result — ""
- seqfil — the name of the pulse sequence
- submit — time of submit action
- start — time the acquisition started
- done — time the acquisition stopped, including data handling, plotting, etc.

The difference between the last two dates is invoiced.

Table header

Enter table headers. For example:

- If `billingmode = goes`,

  Use `tableheaders = "Day" "Time" "Go Rate" "Go/hr"`

- If `billingmode = macros` or `login`,

  Use `tableheaders = "Day" "Time" "Login Rate" "Rate/hr"`

Error Messages

Messages displayed at start up

The software checks if certain items exist at start up and displays error messages if a required item is missing. Only some of the error messages are shown in this section.

If the item exists, the message is as follows:
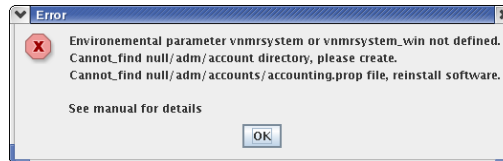
Other messages that are displayed:

- Environment parameter `vnmrsystem` or `vnmrsystem_win` not defined.

- In Linux, this parameter is normally defined in the `.login` or `.cshrc` file using the line: `setenv vnmrsystem /vnmr`

- The line must be added to the `.login` or `.cshrc` file when VnmrJ 3.2 accounting is run by an operating system login (local or remote) account that was not created by VnmrJ 3.2 Admin.

- Cannot find the `nulladm/accounting/accounts` directory, please create.

- This is the directory where the accounts' information is stored. It must exist for the software to store and retrieve the information. In this example, the path starts with null because `vnmrsystem` or `vnmrsystem_win` was not defined either. The correct directory path is `/vnmr/adm/accounting/accounts`.
  Create the path manually if it is not present.

- Cannot find the '`nulladm/accounts/accounting.prop`' file, reinstall software.

- The software needs the properties file to determine logos, currency, and billing mode. The path starts with null, because vnmrsystem was not defined. The correct file path is /vnmr/adm/accounts/accounting.prop. Reinstalling the software is the method to recover this file, unless you can copy it from another place. The file is installed with the VnmrJ 3.2 software.

Account information error message

Times in the rate table must be in chronological order to generate accurate and correct invoices. The software checks that the times in the rate table are in chronological order when the Save button in the account panel is pressed.

A warning message is displayed if the rate table is not in chronological order.
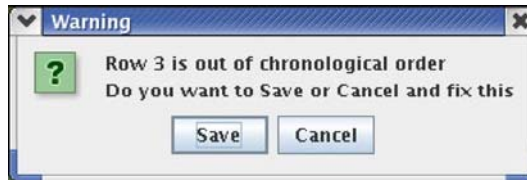
Do one of the following:
- Click the **Cancel** button, correct the order, and click the **Save** button.
- Continue with clicking on the **Save** button — the invoices may not be correct. The software searches for the first entry beyond a login or go time. If the entries are not in chronological order the wrong entry may be used.

Comma separated value (or comma delimited)

Write the printer output to a CSV text file for an individual invoice or all invoices. This file can be imported into an Excel spreadsheet for further processing.

Create the following file to write the printer output to a CSV file:

`/vnmr/adm/accounting/account/CSV_yes`

The file can be a file or directory. Create this file on Linux using:

```
vnmr1>cd /vnmr/adm/accounting/accounts

vnmr1>touch CSV_yes
```

Return to normal printing by renaming the file to `CSV_no` or by deleting the `CSV_yes` file.

Accounting Limitations

- VnmrJ 3.2 Accounting is only run on systems that create billing records. Records are created and invoices generated by the VnmrJ 3.2 Accounting package running on the system where the VnmrJ 3.2 software is installed. Accounts are invoiced by the system. A billing account on multiple systems will have an invoice for each system. Merging records from different systems is not supported.

- Pruning large record files is supported.

- The files `/vnmr/adm/accounting/gorecords.xml` and `/vnmr/adm/tmp/macrorecords` grow larger and larger with time. The VnmrJ 3.2 Administrator must periodically delete records in these files. The `gorecords.xml` file grows the fastest. Use the Properties tab and the Cut Records button to reduce the file size or use any ASCII editor to delete records.

- Billing modes of **Acquisition** (goes) and **Login** (macros) are mutually exclusive. Records for both billing methods can be kept at the same time. Invoices are written based on one or the other mode. Create an invoice using one mode then change the billing mode and create a second invoice in the other mode.

- VnmrJ 3.2 macros write to the `macrorecords.txt` file from different user accounts and set the file access permission to `rw-rw-rw-`. This leaves a lack in the security that allows anyone to modify records. Keep a local copy of the macros that do not write these records.

- `Expproc` writes the `gorecords.xml` file. Access permission for this file is `rw-------`. `Expproc` executes with root permission and does not need general access permission to write to `gorecords.xml`, making it more secure.

8
System Calibrations and Autotest

This chapter describes the liquids NMR system calibration procedures for a newly installed Agilent Technologies, Inc. NMR Spectrometer system. These calibrations and system test procedures can be used for routine system calibration maintenance. Procedures described here cover pulse width calibration, decoupler field strength, decoupler 90° pulse width, and decoupler pulse calibration. Additional calibration procedures are described in various probe installation and acceptance test procedure manuals, accessory test and installation manuals, and other test manuals.

NOTE For more information on manual calibrations, see the *Probes Acceptance Test Procedures*.

NOTE For more information on running AutoTest, see the *AutoTest User Guide*.

Procedure Requirements

- Magnet is installed and ready for normal operation.
- System operating software is installed.
- All required network issues and connections are completed.
- VnmrJ 3.2 software is installed, printers set up, and hardware configuration set.
- All accessories are installed and ready for calibration.

Referenced Manuals

This system calibration procedure references the following manuals:

- *DD2 Installation and Acceptance Test Procedures*
- *400-MR DD2 Installation and Acceptance*
- *Probes Acceptance Test Procedures*
- *AutoTest User Guide*
- *Spectroscopy User Guide*

Calibrating the System

1 Install the primary system probe and complete all the acceptance test procedures.

Typically, this configuration consists of a conventional probe using 5 mm sample tubes, VT system, and gradient(s) (if present). Sample changers, flow systems and probes, cryogenic probe and system, and other specialized accessories are installed and calibrated last.

See Gradient Shimming in the *Spectroscopy User Guide*.

2 Run AutoTest.

See the *AutoTest* manual for instructions and the console acceptance test and installation procedures manual for specifications.

3 Calibrate the probe and create a calibration file.

Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. See "Calibrating a Probe" on page 142 for instructions– choose the calibration procedures that are compatible with the probe functions.

4 Install any additional probes - follow the instructions in the *Probe Installation and Acceptance Test* manual.

5 Calibrate and create a calibration file for each additional probe.

Choose all the calibration procedures that are appropriate for the probe. A new system or probe installation requires the creation of a system level probe calibration file. See "Calibrating a Probe" on page 142 for instructions – choose the calibration procedures that are compatible with the probe functions.

6 Edit the probe calibration file for each probe as necessary and add any manually determined calibrations, for example, add the15N calibrations for an HCN probe.

See "Adding calibrations for 15N calibrations" on page 151.

7 Calibrate any installed accessories such as:

- Cold Probe – refer to the Cold Probe Installation and Cryogenic Systems Installation manuals.

- Sample Changers – refer to the related manual.

- LC‑NMR and LC‑NMR/MS systems – refer to related manual.

- VAST – refer to related manual.

- ProTune – refer to Calibrating ProTune Calibrating ProTune.

Calibrating ProTune

This section applies only to systems equipped with ProTune.

Changing probes

1 Remove the current probe – do one of the following:

Currently installed probe is a ProTune or PZT compatible probe.

a Eject the sample if one is present.

b Turn OFF the master module or probe tuning controller.

c Disconnect cables to ProTune controllers from the probe.

d Remove the RF cables and pneumatics lines.

e Remove the probe from the magnet.

Currently installed probe is not a ProTune or PZT compatible probe.

a Eject the sample if one is present.

b Remove the RF cables and pneumatics lines.

c Remove the probe from the magnet.

2 Install the next probe in the magnet.

3 Set the system probe name to the currently installed probe.

4 Do one of the following:

Installed probe will use ProTune or PZT.

a Connect flexible shafts or controller cable to the probe.

b Connect the RF cables and turn the Master module or probe tuning controller ON.

c Set or verify that the system hardware option, ProTune, is set to **present**. See "Spectrometer configuration" on page 25.

Installed probe will not use ProTune or PZT.

a Set system hardware to ProTune not present, see "Spectrometer configuration" on page 25.

b Connect all cables and pneumatics lines to the probe.

Connecting ProTune modules to the probe

1 Connect the cables from the ProTune module to the probe in the order shown, using the procedure in the next step.
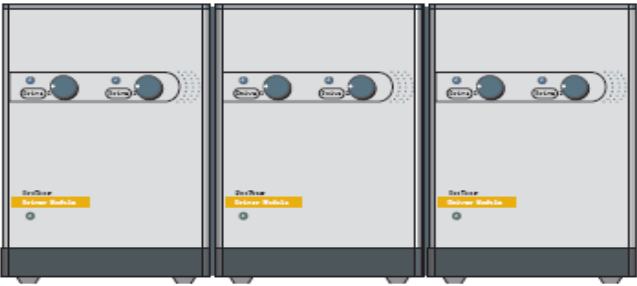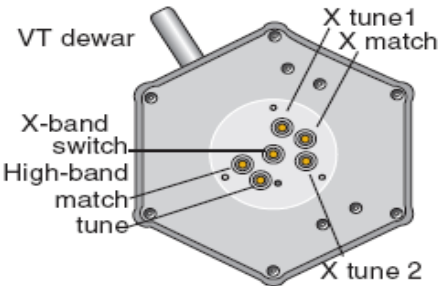
AutoX Probe Capacitor	Master	Drive Module 1	Drive Module 2
X-band Switch	—	—	Drive 1
X Tune 1	—	—	Drive 2
X Match	—	Drive 1	
X Tune 2	—	Drive 2	
High-band Match	Drive 1		
High-band tune	Drive 2		

2 Connect each cable from the ProTune modules to the probe as follows:

a Align the slot on the cable end with the pin on the knob of the probe.

b The slot (A) lines up with the set screw (B) on the flex shaft.

c Push the shaft on to the knob and compress the spring in the knob.

d Turn the capacitor knob approximately 90º clockwise to lock.

e Repeat this procedure for each capacitor and cable pair.

Connecting the probe tuning controller to the probe

Connect the cable from the Probe Tuning Controller to the Probe Tuning Module Driver with the red dot on the connector cable facing up.

Motor Index

This section applies only to those systems equipped with ProTune or PZT. The ProTune or PZT motors might need to be indexed after the following:

• The probe has been changed.

• The Master Driver Module or probe tuning controller has lost power, has been power cycled, or is going through initial installation.

| NOTE | The motors will be automatically indexed with the current probe if power to the controlling unit has been interrupted since the last time the ProTune command was executed. |

Indexing all the ProTune motors and PZT

1 Log in as administrator, typically vnmr1.

2 Set the system probe name to the name of the currently installed probe.

3 Verify if all ProTune connections are correct.

4 Turn the ProTune modules On and the system is Idle.

5 Type `protune('calibrate')` at the VnmrJ 3.2 command line.

The ProTune Interface window appears.
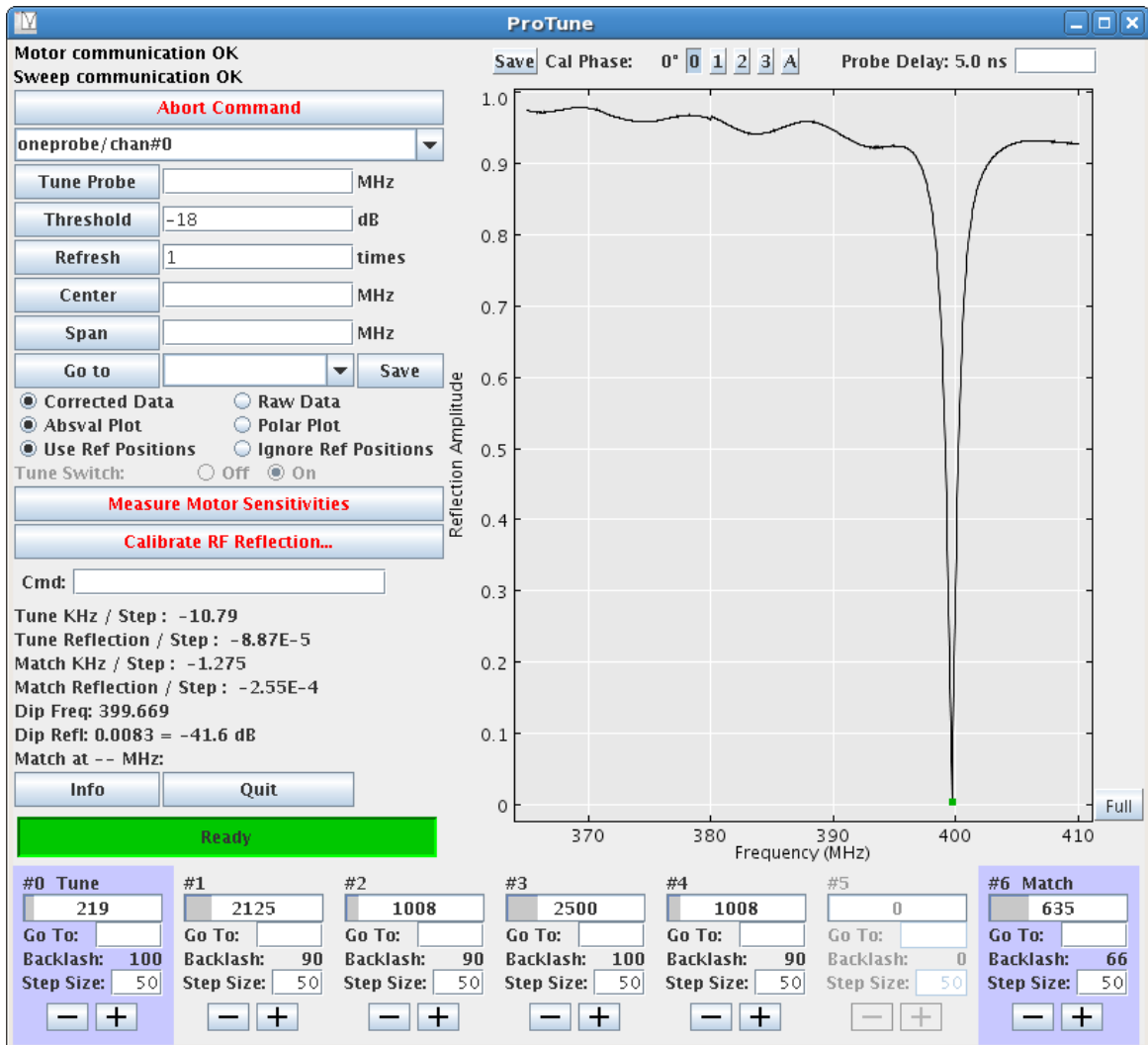
Figure 10   ProTune GUI

6 Verify that the Motor and Sweep communication show **OK**
in the top left corner of the ProTune Interface window.

7 Type `index all` in the ProTune window Cmd field.

Each motor will be indexed automatically. Wait for the indexing process to complete.

8 Exit from the ProTune Interface.

Indexing individual ProTune motors

1 Log in as administrator, typically vnmr1.

2 Set the system probe name to the name of the currently installed probe.

3 Verify all ProTune connections are correct.

4 Turn the ProTune modules On and the system is Idle.

5 Enter `protune('calibrate')` on the VnmrJ 3.2 command line.

The ProTune Interface window appears.

6 Verify that the Motor and Sweep communication shows **OK** in the top left corner of the ProTune Interface window.

7 Enter `index <motor number>` in the ProTune window Cmd field, see Table 18.

The motor will be indexed automatically.

Table 18   Module and motor designations

	Master module		Dual module 1		Dual module 2	
Alternate name	**Box 1**		**Box 2**		**Box 3**	
Motor number	1	0	3	2	5	4
Drive number	1	2	1	2	1	2
Probe connection	HB Match	HB Tune	X Match	X Tune 2	X Switch	X Tune 1

8 Wait for the indexing process to complete.

9 Repeat steps 7 and 8 for next motor to be indexed.

10 Exit ProTune Interface.

Clearing motor stuck message with ProTune (not PZT compatible probe)

The software displays the motor stuck warning if the indexing process does not reach an end or if the motor cannot turn the capacitor. The message will specify a box or a motor number or both. See Table 18 for module and box number correlation. Clear the error message using the following procedures:

1 Indexing does not reach an end.

    a Check and tighten all the screws on corresponding flexible shaft. Use the non-magnetic tools provided with ProTune Tool Kit.

    b Re-index the motor.

2 Tune knob is stuck.

    a Disconnect flexible shaft from the probe's tune knob. Use the non-magnetic tools provided with ProTune Tool Kit.

    b Use the tuning stick provided with the probe and turn the knob in the opposite direction as indexing to free the knob.

    c Re-connect flexible shaft and re-index the motor.

Calibrating Sweep Range

This section applies only to systems equipped with ProTune or PZT. The sweep range must be calibrated if parts of the RF path, cables or filters, are changed. Sweep range calibration is probe independent.

Calibrate the ProTune sweep range by measuring the RF reflection using the following procedure:

1 Log in as the VnmrJ 3.2 administrator (typically vnmr1) and start VnmrJ 3.2.

2 Type `ProTune('calibrate')` at the VnmrJ 3.2 command line.

The ProTune Interface window is displayed.

3 Verify that for both Motor and Sweep communication **OK** is displayed (upper left corner of the window).

4 Click the **Calibrate RF Reflection** button.

The following pop-up wizard appears. Choose High Band or Low Band, the sweep width is set for you. Then, click **Next** to continue.

5 Follow the directions in the subsequent pop-ups to complete calibration of the selected band.

6 Repeat steps 4 through 6 for the other band.

Calibration verification

Verify the calibration of this channel as follows:

1 On the commad line, type the command `setCalSweep` along with the sweep range to check. For example, the range for the low band from the graphics above is 30 to 185 MHz; so, the command `setCalSweep 30 185` is entered.

2 A flat line at `reflection=1` is the ideal response.

Exiting the calibration mode

1 Remove the shorting plug and reconnect the probe.

2 Connect the proton and X channels to the probe.

3 Close the **ProTune Interface** window.

Calibrating a Probe

This procedure uses the VnmrJ 3.2 Spectroscopy interface. A complete list of samples and calibration tests are in AutoCalibration.

Logging in and installing the probe

Completion of these steps is required for all the procedures that follow.

1 Log in to VnmrJ 3.2 as the administrator, typically vnmr1, to create a system probe file (typical for initial installation).

NOTE	Write permission to `/vnmr/probes/probe_name` is required to create a system level probe file

2 Install the probe to be calibrated.

Probe installation instructions are provided in the *Installation and Operations* manual for the probe.

Setting up, selecting, and creating a probe calibration file

To create the probe calibration file before calibrating a probe for the first time, use the procedure described below.

1 Click the **Probe** button in the hardware bar of the VnmrJ 3.2 interface or click **Tools** on the VnmrJ 3.2 menu bar, select **Standard Calibration Experiments**, and select **Calibrate probe**.

The probe selection window appears. See Figure 15 on page 153.

2 In the **Manage Probe Files** section of the probe popup window, type the new probe name into the field for Probe name (letters first, followed by numbers and no spaces, e.g. abc456) and press the Return key.

3 If ProbeID is installed on the system, from the **Probe ID** pull-down menu choose either **Probe without ID** to create a

blank probe file or choose the probe ID that corresponds to the desired probe to create a probe file that is pre‑populated with approximate calibration values for that style of probe.

4 Do one of the following based upon the operating system login:

- VnmrJ 3.2 system administrator (typically vnmr1) or user with equivalent write permissions – select the appropriate radio button to choose either:
  Systemdir— writes the calibrations into:
  `/vnmr/probes/probe_name`
  and makes all calibration available to all users — typical for new system and probe installation.
  – OR –
  Userdir — writes the calibrations into:
  `~/vnmrsys/probes/probe_name`
  and is available only to the logged in user creating the calibration file.
  The User level calibration file can be written to the system level directory, if the user has write permission to the system level directory, by entering the desired file name and clicking **Copy**. See Figure 15 on page 153.

- Logged in as a user (most users) without write permission to `/vnmr/probes` files.

- Continue with the next step – the Level option is not displayed and all calibrations will automatically be saved to `~/vnmrsys/probes/probe_name`.

5 Click the **Create** button.

a Do the following for nano and AutoMAS probes:
Enter `tach` in the field next to Probespintype (do not use the nano option).
Enter an approximate maximum spinning speed based on the probe:
Nano probe — 2500 is typical
MAS probes — Maximum value for the spinner that will be used most often. Refer to the probe manual for specifications of spinner speed, material, and temperature.
Update the parameters after adding an MAS type probe

by entering `probe=probe` on the VnmrJ 3.2 command line. Selecting the new MAS type probe will now automatically set the spintype and the maximum speed. The Spin/Temp panel will require updating if it was open while the new probe was added. Select any other panel then select the Spin/Temp panel.

b Continue with "Starting a calibration" on page 145.

Existing probe

a Select the probe from the drop-down menu.
If this probe file was NOT created from VnmrJ 3.2, then the probefile should be updated so that it will contain additional parameters for use in VnmrJ 3.2. Take note of the lock power and lock gain values stored in the probe file.
Click **Edit**, then click the **lk** tab in the Probe edit window, then from the command line type `updateprobe` to update the probe. Then, re-enter the lock power and gain values for the various solvents in the probe file.

NOTE	The new/updated probefile will contain the parameters `Probewtune` and `Probetunemethod`. If the probe is a ProTune-compatible probe, these parameters should be set for the desired operation. The directory `/vnmr/tune/methods` contains the entries valid for `Probetunemethod`. The parameter `Probewtune` takes the same parameters and has the same usage as the parameter `wtune`. (See the *Command and Parameter Reference* entry for wtune.)

b Continue with "Starting a calibration" on page 145.

Tuning probes

Probe tuning is covered in the *NMR Spectrometer User Guide*. Tuning operations and tuning ranges specific to each probe are covered in the manual provided with the probe.

Starting a calibration

1 Click the **Setup Calibration** window in the **Probe** window.

2 Select **Calibrations** from the Calibration pop-up window.
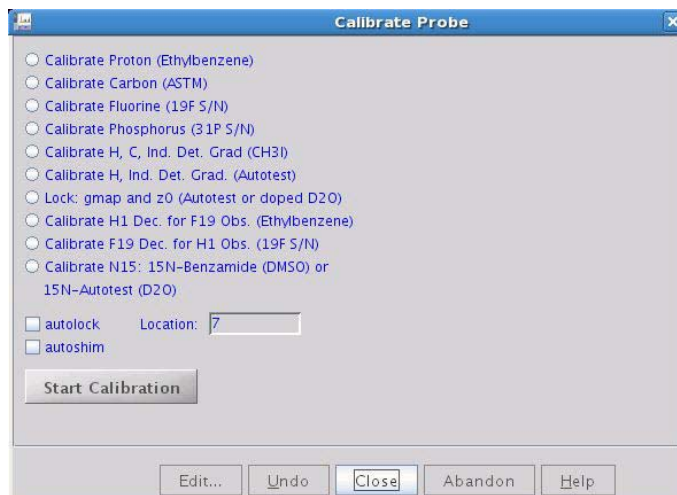
a Click an option button in the calibrate probe window to select the calibration experiment.

b Enter the location of the calibration sample.
No entry field appears if a sample changer is not attached to system.

c If a sample change system is not present or not used, insert the sample into the magnet manually using the Insert and Eject buttons. It is located on the Lock page of the Start tab.

d Select the **autolock** check box to have the system automatically lock the sample.

e Clear the **autolock** check box if your sample is already locked or if you would prefer to lock manually.

f Select the **autoshim** check box to have the system automatically shim the sample.

g Clear the **autoshim** check box if the sample is already shimmed or to shim manually.

3 Follow the procedure in "AutoCalibration" on page 157 for the autocalibration procedure that was selected in step 2a.

- Verify the correct sample is present in the probe. Probe calibration will begin.

- The calibration files are created and written to the locations determined by the level that was selected in "Setting up, selecting, and creating a probe calibration file" on page 142.
  Some probes, like the Autoswitchable and 4 nucleus probes, require additional calibrations not covered in this manual. For information on the calibration of these probes, see the Installation and Operations manual for the probe.

4 Select **autoshim** to have the system automatically shim the sample.

5 Click the **NO** button if your sample is already shimmed or if you would prefer to shim manually.

Starting a calibration in Experiment Selector

In VnmrJ 3.2, probe calibration tests are accessible in two locations:

- **Probe window > Setup Calibrations**.

- In Experiment Selector on the new Calibration tab: **Experiment Selector > Calibration**.

Performing calibrations from the Experiment Selector, allows the calibrations to be run similar to a study: foreground mode or automation.

Running calibrations as a study:

- allows a complete record of acquired data to be kept in the study folder
- allows for effective troubleshooting
- updates probe files with new values at the end of a calibration

Using the Calibrations tab

The Experiment Selector is located on the left-hand side of the standard VnmrJ interface under the Protocols tab.
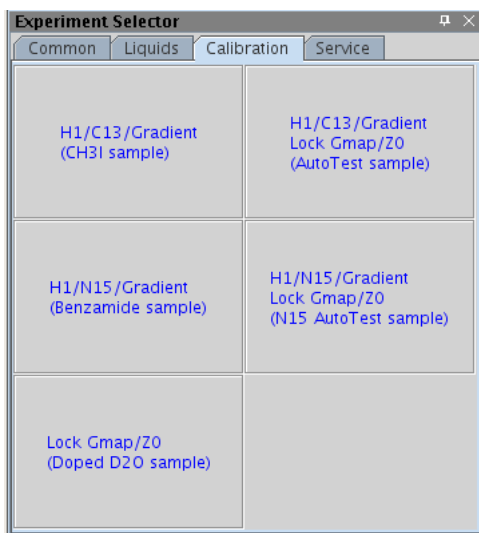
Figure 11   Experiment Selector-Calibration tab

1 Select the Calibration tab in the Experiment Selector to view the available studies. Five studies are currently available, each of which correspond to a specific standard calibration sample.

2 Select **New Study** from the Study Queue panel in the bottom left.

3 Select the Calibration experiment for the sample to load the experiment into the study.

The Acquire tab now has two panels loaded: selected standard sample and Overview. The Overview panel is simply a parameter display. The top panel shows a list of calibrations available for the chosen sample and a few key parameters.
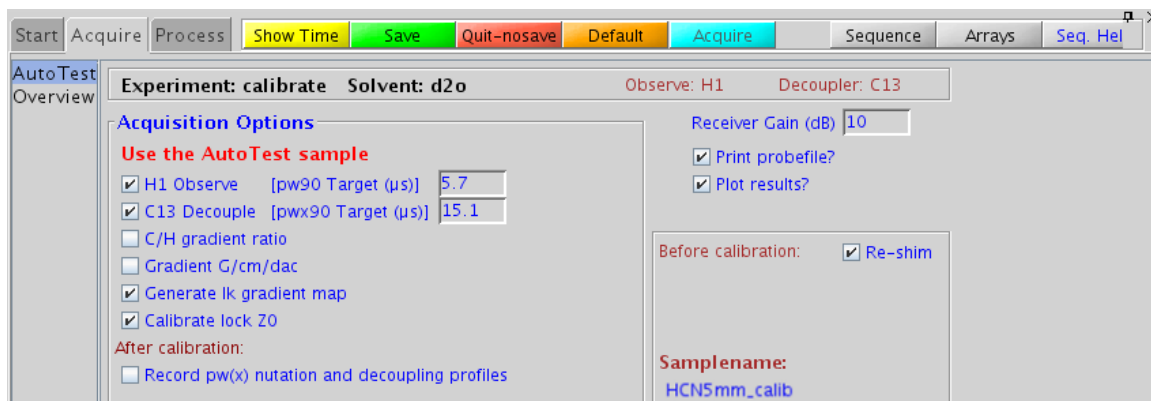
Figure 12   Acquire tab displaying selected Calibration experiment.

4 Select Acquisition Options for the selected calibration. Enter a target 90° in µs for pulse calibrations.

5 Enter the receiver gain to the right of the panel.

6 Select whether to print the probe file and plot the results after the calibration.

7 Select whether to re-shim the sample before calibration.

8 Select whether to to record the nutation and decoupling profiles for subsequent review in the bottom left of the panel.

9 After selecting the desired experiments, parameters, and output, click **Submit** to submit the calibration study to either the foreground or background automation. The appropriate experiments will be placed in the Study Queue.
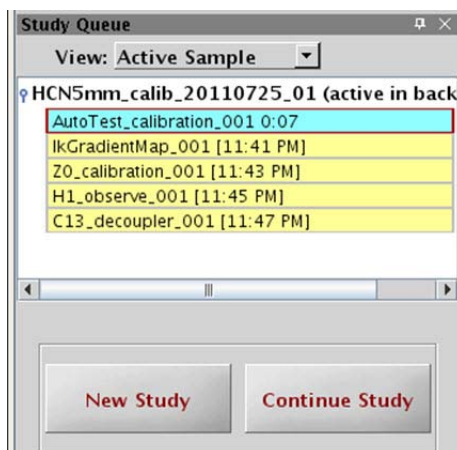
Figure 13   Submitted calibration experiment in Study Queue.

Submission to background automation allows for calibration to be run unattended at night, or even in the middle of long automation runs for QC purposes. Or, if the current VnmrJ user is allowed to select to sample position, a standard sample can be stored in a seldom-used position of the autosampler to allow for quick calibrations at any time.

The probe file is updated automatically at the end of each calibration with the new value(s). Data and parameters are stored in the study file. If multiple arrays are used for pulse calibrations, these will be saved separately. The data can then be readily accessed from the study queue and examined for easy troubleshooting should any of the calibrations fail. The calibration study file also can provide a record of the calibrations for labs that may require documentation of regular QC for regulatory purposes. Figure 14 displays an example of output from a CH3I calibration.
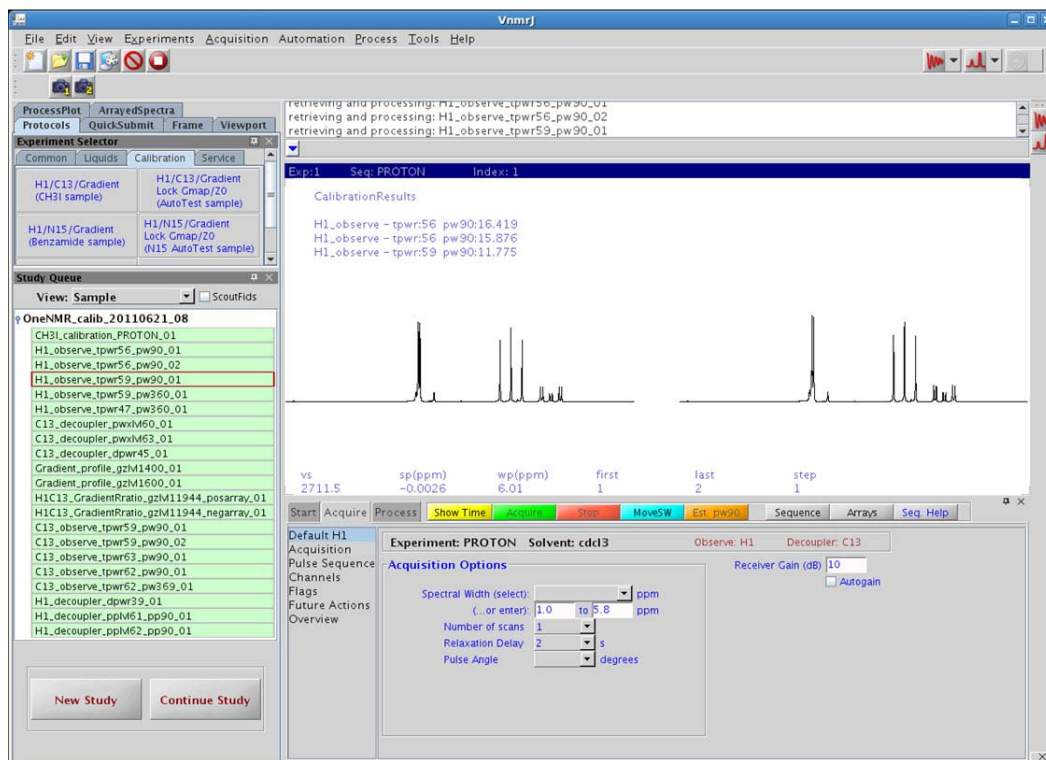
Figure 14   Example of calibration study file output from a CH$_3$I calibration.

Adding calibrations for ^{15}N calibrations

The calibrations for ^{15}N can be added to the probe calibration file following the manual calibration for probes with an X channel that can tune to ^{15}N or that have a pre-tuned ^{15}N channel.

To add Calibrations for ^{15}N:

1 Click the **Probe** button on the hardware bar in the VnmrJ 3.2 interface, or

2 Click **Tools** on the VnmrJ 3.2 menu bar, select **Standard Calibration Experiments**, and select **Calibrate** probe.

3 Select the **Edit** check box — editing options appear in the Probe window.

4 Click the **Select Probe File** drop-down menu and select the probe.

5 Click **Edit Probe File**.
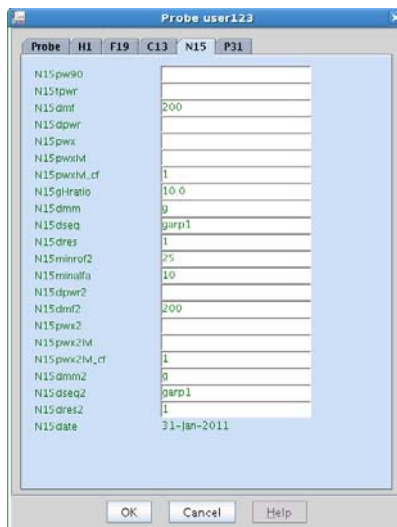
A pop-up window appears with calibration names and fields to enter values.

6 Select the **N15** tab.

7 Add the calibration values in the provided fields – current calibration values are next to the parameter name, for example, pw90 (14).

Leave the field empty if a calibration is not available – do not enter a zero.

8 Click **Save**.

9 Click **Exit**.

Viewing or editing calibration values

Each of the probe calibration files can be viewed and edited. Editing individual parameters is best done at the user level probe file and not at the system level. This is appropriate for specialized calibrations such as high salt concentrations, biological samples, and low temperature calibrations etc. that are specific to an individual user but not appropriate for all users.

To edit or view a calibration value:

1 Click the **Probe** button in the VnmrJ 3.2 interface or click the **Utilities** button in the VnmrJ 3.2 menu bar.

2 Select **a probe** from the Select Probe drop-down menu.

3 Select **the check box** next to Edit.
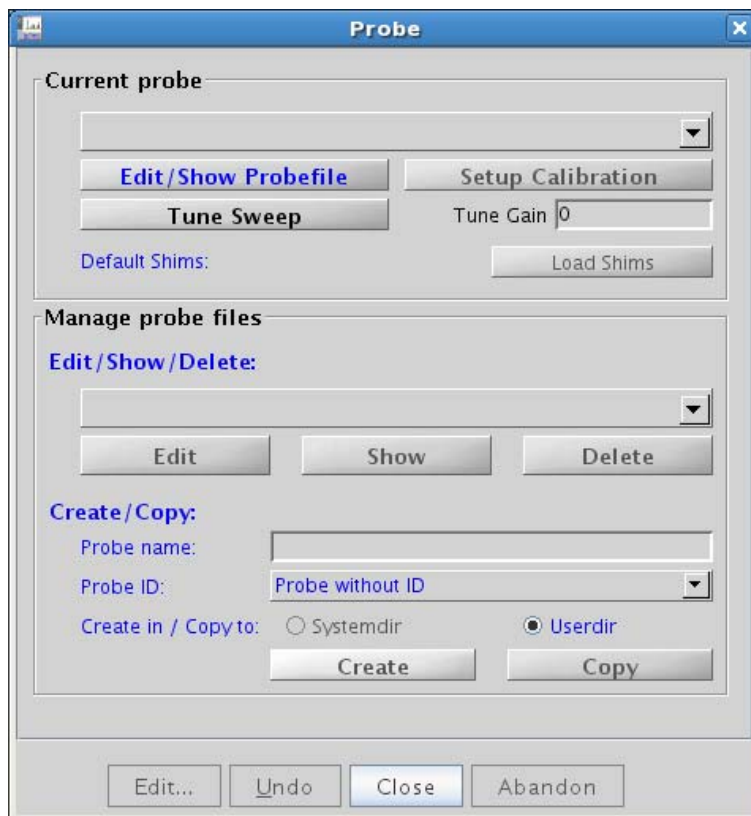
Figure 15   Calibrating a probe

4 Check the **Edit** button—editing options appear in the Probe
window, see Figure 16.
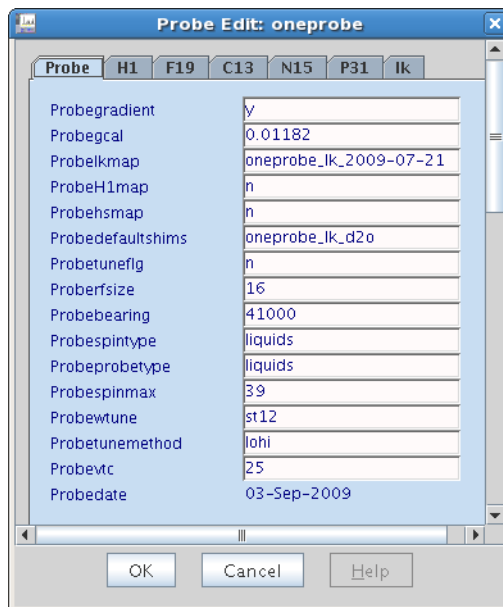
Figure 16   Probe file edit window

5 Select the tab to modify a probe calibration entry.

6 Change the calibration values in the fields provided.

Leave the field blank if a calibration is not available — do not enter a zero.

7 Click **OK**.

8 Click **Exit**.

9 Repeat for each probe calibration file as required.

10 Click **Close** to exit the Probe calibration pop up window.

Optional – create a new version of the probe calibration file that will contain any special calibrations (typically a user level requirement):

1 Open a terminal window.

2 Do one of the following:

   • User level probe file:
     Type `cd ~/vnmrsys/probes`
     – this is the probes directory of the current operating system log in user.

   • System level probe file:
     Type `cd /vnmr/probes`.

3 Copy the directory for the probe of interest to a new directory name.

4 Change directories to the probe name directory.

5 Rename the probe file in the directory to exactly the same name as the directory.

AutoCalibration Samples

The samples listed in Table 19 can be used for auto calibration. Not all samples are provided with each system. The required samples for the acceptance test procedures during system installation will include one or more of these samples.

Table 19   AutoCalibration samples

Sample	Calibrate option	Part number
0.1% ethylbenzene in CDCl3 1H sensitivity	Proton	00-968120-70
40% dioxane in C6D6 13C sensitivity	Carbon	00-968120-69
0.485 M triphenylphosphate in CDC13 31P sensitivity	Phosphorus	00-968120-87
0.05% trifluorotoluene in benzene d6 19F sensitivity	Fluorine	00-968120-82
1% ^{13}C-enriched methyl iodide, 1% trimethyl phosphite, and 0.2% Cr(AcAc) in Chloroform-d	Proton, Carbon, ID, and Gradients (organic solvents)	00-968120-96
0.1% 13C-enriched methanol, 0.1% ^{15}N-enriched acetonitrile, and with 0.30 mg/ml GdCl3 in 1% H2O/99% D2O (AutoTest Sample)	Proton, Carbon, ID, and Gradients (aqueous solvents)	00-968120-68

AutoCalibration

1 Click any one of the following **calibration option** buttons:

- Calibrate Proton (Ethylbenzene)
- Calibrate Carbon (ASTM)
- Calibrate Fluorine (19F S/N)
- Calibrate Phosphorus (31P S/N)
- Calibrate H, C, Ind. Det. Grad (CH3I)
- Calibrate H, C, Ind. Det. Grad (Autotest)
- Lock:gmap and z0 (2Hz D2O)
- Calibrate H1 Dec. for F19 Obs.(Ethylbenzene)
- Calibrate F19 Dec. for H1 Obs. (19F S/N)

2 Follow the prompts, enter any required values, select options, and proceed according to the instructions presented in the Calibrate probe window; see Figure 17 for an example of the prompts presented.

3 Click the **Start Calibration** button.
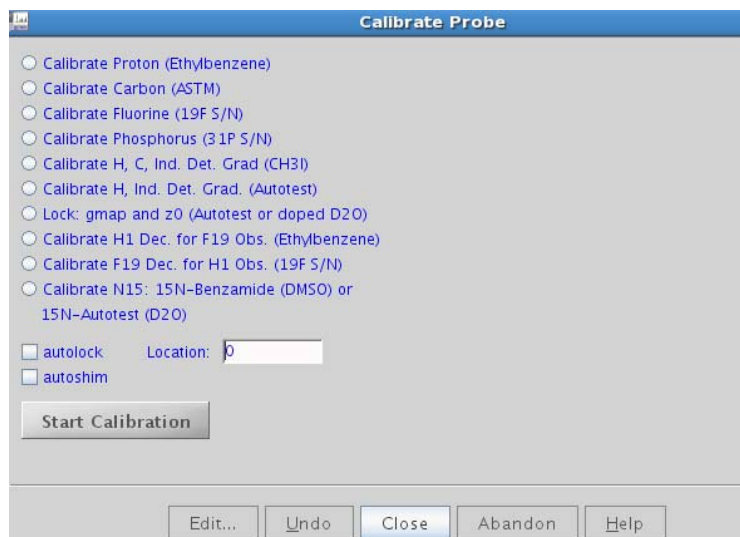
Figure 17   Calibrate probe

Running AutoTest

Refer to the *AutoTest User Guide* for details on how to run and work with AutoTest.

A
VnmrJ 3.2 Terms
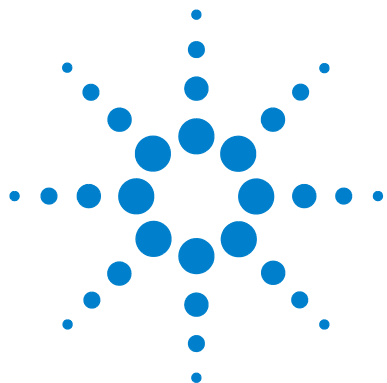
Liquids

Account-Owner, account-administrator or user

Account-owner, administrator or user is the user that owns the operating system login account. User privileges include access to the command line, all parameter panels and all protocols, and right to create new or edit protocols for operator use. The user (account owner) is the head of a group of operators that share the particular login account. User responsibilities include maintaining special protocols and probe files for this group of operators.

Acqlog

The acqlog file (in `/vnmr/tmp`) allows the spectroscopist to monitor an automation run as it progresses in background. The `acqlog` is a simple text file that (if it exists) is updated automatically as a study is submitted to the acquisition queue or Study Queue.

Application directory

VnmrJ 3.2 application directories are directories where VnmrJ 3.2 looks for directories such as `templates`, `maclib`, `manual`, `menulib`, `parlib`, `probes`, `seqlib`, `shims`, `tablib`, `shapelib`, `gshimlib`, and `mollib`. These are directories that VnmrJ 3.2 uses during its normal operation.

Application type

Application types (`apptype`) define how related experiments or a family of experiments, are set up, acquired, processed and plotted.

Background acquisition

A background VnmrJ 3.2 process is spawned for this acquisition when one or more experiments are submitted for acquisition from the Study Queue if background or automation is selected. All workspaces are available for data analysis while VnmrJ 3.2 collects NMR data in a background process.

DayQ

The DayQ is typically between the hours of 8:00 a.m. and 6:00 p.m. and provides 30 minutes of NMR time for each sample submitted by the operator. Submitted samples are accepted to the DayQ provided the sample data acquisition time does not exceed the time limit. See also NightQ.

Direct acquisition

Direct acquisition is carried out as a foreground acquisition and the Study Queue is not used. Select an experiment/ protocol from the vertical experiment panel in direct acquisition mode or from the list of experiments accessed by clicking **Experiments** on main menu. Parameters are loaded directly into the current workspace for manual data acquisition.

Experiment

See "Workspace " on page 167.

File types

NMR data sets have the file extension .fid. The .fid file (FID free induction decay data) contains all of the raw data and parameters of an acquired data set.

A parameter file or set has the .par extension and contains the parameters necessary to set up and acquire an NMR experiment. Parameter files may be both local and global.

A shim file contains a list of shims and their values. Both .fid directories and .par directories contain a file called `procpar`, which includes the shim settings.

Foreground acquisition

When working in direct acquisition mode, the workspace is tied to a particular manual acquisition. No other NMR data set may be loaded into the active workspace while data acquisition is in progress.

Minimize spectral window

The minsw (minimize spectral window) process is often executed before a 2D experiment. First a full spectral width 1d is acquired. The software detects where the highest and lowest field peaks are, recalculates the spectral width, and reacquires the 1d experiment with the new spectral width. The `minsw` process is automatically turned on if a `proton`, `preset`, or `wet1d` protocol precedes a 2D protocol.

NightQ

The NightQ is typically between the hours of 6:01 p.m. to 7:59 a.m. and provides 3 hours of NMR time for each sample submitted by the operator. Submitted samples are accepted to the nightQ provided the sample data acquisition time does not exceed the nightQ time limit. See also DayQ.

Operator

The administrator (vnmr1) creates operators as subservient users of a particular user's account. The operator does not own the login account. The operator may be considered a spectroscopist within a group where the group's head owns

the login account. The operator privileges such as limited access to parameter panels (`panellevel`), command line, or NMR experiments are defined by the VnmrJ 3.2 administrator.

Panel level

The VnmrJ 3.2 parameter, `panellevel`, defines the number of pages an operator has access to in the horizontal panels. The VnmrJ 3.2 administrator (vnmr1) determines the panellevel for each operator.

Probe file

A probe file is a list of parameters that change with each probe: pulse widths, powers, decoupling patterns or shapes for proton, carbon and other nuclei (if applicable). The probe files are maintained in either local directories or globally in the probes directory of /vnmr. Users have a local probe file (vnmrsys/probes) that they keep current with the latest calibrations and gradient shimming files. The global probe file is maintained by the administrator's (vnmr1). A probe file that corresponds to the installed probe must be selected for proper functioning of protocols within VnmrJ 3.2.

Priority sample

A priority sample is submitted to the Study Queue by checking the Priority Sample box before submission. The sample is run after data acquisitions for current sample is completed, and before the other samples submitted to the Study Queue are run. The ability to run a priority sample can be assigned to an operator by the VnmrJ 3.2 administrator.

Protocol

A protocol consists of any single or series of NMR acquisitions. A protocol may be a simple NMR experiment or involve a series of shorter acquisitions that are acquired but not stored in order to establish necessary parameters (such as solvent location) for the desired NMR experiment.

Required experiment/protocol

A required experiment/protocol is an experiment/protocol consisting of one or more required experiments that are executed before the desired data set is acquired. All 2D protocols in the walkup interface require that a proton `apptype` protocol is run before the 2D protocol is run. Selecting a 2D protocol, such as the `Cosy` protocol, automatically adds a proton protocol ahead of the 2D protocol. The requirements for running a proton `apptype` protocol is met if a proton `apptype` protocol (`proton`, `preset`, or `wet1d`) already exits in the list of experiments before the 2D. A required proton experiment, that is part of the 2D protocol, is not added to the Study Queue. Solvent suppression parameters are carried forward to the 2D experiment if the proton `apptype` protocol is `preset`, or `wet1d` and the 2D experiment is acquired with these parameters. A `minsw` process executed if `proton`, `presat`, or `wet1d` listed ahead of any 2D experiment and, if it is not desired, must be turned OFF before the experiment is submitted.

Spectroscopy interface

The walkup is primarily designed for point and click acquisition of NMR experiments with or without a sample handler (SMS, Carousel, VAST, 768AS).

Study

A study consists of a one or more NMR experiments collected on one or more NMR samples.

Study Queue

The Study Queue is an area in VnmrJ 3.2 where a list of protocols (NMR experiments) to be acquired on a single sample or a series of samples is created. This area can reflect the sample that is active, the sample that is displayed, or a queue.

Traymax

The parameter traymax is used define the type of autosampler or sample handler associated with the NMR system and can have the following values.

traymax =	Sample handler
0	No sample handler
1	LC-NMR or LC-NMR/MS
9	Carousel
12	7510-AS
50	SMS with a rack for 50 samples
100	SMS with a rack for 100 samples
96	VAST
97	7600-AS
768	768AS robot

Viewport

Activating viewports allows the user to view more than one workspace at a time. Each viewport must be linked to a specific workspace. Up to nine viewports can be open in VnmrJ 3.2 at a time. Viewports allow the user or operator to look at one or more spectra (with or without linking cursors) at a time.

Workspace

The terms workspace and experiment are used interchangeably. Either one refers to a directory in the user's local vnmrsys directory called `exp1, exp2, exp3,` etc., which correspond to workspace 1, workspace 2, workspace 3, or equivalently, experiment 1, experiment 2, experiment 3 and so on. The exp directory contains parameters and, potentially, data for any given NMR experiment or protocol.

Data is directly acquired into a defined workspace or experiment corresponding to an exp directory in direct acquisition mode and must be stored into a FID file or it will be overwritten by the next direct, user-executed acquisition. The workspace or experiment can also act as a holding pen for processed data that is already stored on the disk.

Imaging

Applications type

Experiments are grouped in types of applications such as: 3D fast spin echo, localized spectroscopy (1D), global spectroscopy (1Dglobal), or EPI-like. Each application type has, a generic set-up, processing, and prescan procedure.

Composite protocol

A composite protocol is a series of protocols, required protocols, prescans, or a series of NMR data acquisitions, clustered together into one unit.

Exec-parameters

The exec-parameters (string parameters) define how a particular protocol is prepared for scan (execprep), processed (execprocess), or run in the prescan mode (execprescan). Typically, the exec-parameters contain just the name of a single macro, but generally they can be anything that could be typed on the command line or typed in a macro.

File types

Spectroscopy data is stored with the raw data is saved a single file (fid) accompanied by an ASCII file listing all parameters in the subdirectory name.fid. Image data is stored with the processed images saved as individual files for each slice in a 2D experiment or as a single file in a 3D experiment in the subdirectory `name.fdf`.

Protocol

A protocol can either be a basic or composite. A basic protocol is a single parameter set, for example, sems or gems, whereas a composite protocol is a collection of basic protocols.

Study

A study consists of one or more scans run on a single subject in a single session.

Study queue

The Study Queue is a list of protocols to be acquired. These protocols are coded with different colors and fonts to distinguish between active, completed and new protocols. The protocols move to the top as scans are acquired.

Viewport

There are usually three available Viewports: Plan, Current, and Review. Each viewport is a separate work-area with different functions. Use the Plan Viewport to set up experiments and graphically plan the slices or volume. The data will be acquired and displayed in the Current Viewport, which therefore always has the most recent data. Use the Review Viewport to view and analyze previously acquired data.

Administrator

Administrator (vnmr1)

The administrator of VnmrJ 3.2 (both hardware and software) is generally called vnmr1 and is the owner of all files and directories of the VnmrJ 3.2 software. Typical functions of the VnmrJ 3.2 administrator are: creating new users and operators, assigning appmodes and various privileges such as access to panels and NMR experiments, and hardware configuration through the vnmr1 user login.

Application mode (appmode)

The application mode determines what features are displayed in the VnmrJ 3.2 window. The application modes are Spectroscopy, LC-NMR and Imaging. The administrator (vnmr1) defines each user's application mode upon the creation of that user's operating system login account.

General

Folder

The user interacts with the parameters through panels in one of the four folders: Start, Acquire, and Process. Each folder can have a number of pages. The folders are found in the bottom horizontal region of the VnmrJ 3.2 interface.

Global files

Global parameters, templates, experiments, file and so forth are available to all users and are stored in the /vnmr directory, which is owned by the system administrator (vnmr1).

Local files

Local files (parameters, templates, experiments, probe files, and so forth) are stored in the user's directory (~/user/vnmrsys). Local files typically are specified as the first application directory to search.

Locator

The locator is a database manager that helps spectroscopists keep track of the location of automation runs, shim files, protocols, acquired data and so forth.

Node in study queue

Each entry in the study queue is termed a node. A node is either a parent node (the name of the sample or a child node (the actual scan).

Pages

The sub-panels in each folder are called pages, panels, or templates. These pages have entry fields, menus, check boxes, and so on, for setting up sample-specific, acquisition, or processing parameters.
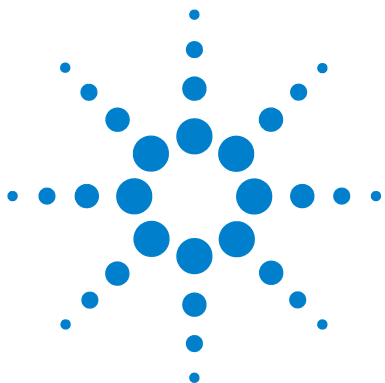
Prescan(s)

A prescan is a short acquisition generally not saved to disk that can be part of or precede protocols. Prescans that are integrated into protocols include solvent suppression optimization routines (presat in 90% water), and scout scans to find solvents for suppression. Prescans that precede protocols or data acquisition are automatic tuning, locking and gradient shimming. These prescans are set-up from the "Standard" page found in the "Start" folder.

Push-pin

A small icon that looks like a tack or a push-pin is located in the upper right of the folders and vertical panels. By untacking the push-pin, the user can hide the folders or vertical panels. A tab to the side of VnmrJ 3.2 is created. When the mouse is rolled over the tab, the vertical panel or folder will be temporarily redisplayed. If permanent redisplay of the panel or folder is desired, the push-pin may be tacked in place.

Vertical panels

The vertical panels are located on the left-hand side of the screen. They provide easy access to general cross-applications functions, which is particularly useful when the horizontal folders are hidden.

B
Printers and Plotters Troubleshooting

This appendix contains troubleshooting and setup information for printers and plotters. It describes a number of printers and plotters tested as compatible with VnmrJ 3.2. Check the Agilent website for new printers that work with VnmrJ 3.2. Refer to the original system manuals supplied with the printer or refer to the on-line manuals for printers supplied with older spectrometers.

Agilent Technologies

Hewlett-Packard LaserJet 840C Printer

Printer I/O	HP IEEE-1284-B Parallel
	Universal serial bus
	1284-B receptacle
Printer language	HP PCL 3
Printer memory	2 MB standard memory
Cartridges	black and color
Resolution	Black – 600 x 600 dpi with black pigmented ink
	Color – HP color layering technology
Pages per minute	Black – 4 ppm
	Black and color – 0.8 ppm
Configuration control	Software controlled

There are two buttons and three lights on the front panel of the printer. The lights indicate if the printer is operating correctly or indicate the time when the printer requires attention from the user.

Self-Test procedure

Turn the HP DeskJet 810C and 830C series printer off and remove the cable that connects the printer to the computer.

Turn the printer back on.

Press and hold the **Power** (top) button. Press the **Resume** button 4 times and then release the **Power** button.

The self-test page will print with a report containing the printer model name, serial number and a diagonal self-test pattern. The test pattern verifies that all nozzles on the print cartridge are firing. If a gap appears along the diagonal self-test pattern, one or more nozzles are not firing.

Operation

Turn off the power.

Connect the interface and power cables.

Press **Go** to turn the power on. The ready light should come on.

Open a terminal window, log in as root, and activate LaserJet_150, LaserJet_150R, LaserJet_300, LaserJet_300R, LaserJet_600, and LaserJet_600R using the procedures in the beginning of this chapter.

Set the parameter printer, from within VnmrJ 3.2, to the name you typed in the previous step, for example, printer=`'LaserJet_300'` or printer='lj'. Type `printon dg printoff` to produce a test print.

To use as a plotter, set the parameter plotter to the name you typed in the previous step, for example, `plotter='lj 300'` (If you activated more than one resolution, there will be different names corresponding to the different resolutions). To test, type `pl page`.

Lexmark Optra Color 45 Inkjet Printer

Printer I/O	IEEE 1284 ECp compliant,1284-B receptacle, Internal Solutions Port (6 options).
Printer language	PostScript Level and PCL 5c emulation.
Printer memory	8 MB.
Cartridges	Dual head thermal inkjet
Resolution	600 x 600 dpi
Pages per minute	Black - 8 ppm
	Color - 4 ppm
Configuration control	Software controlled

The Agilent supplied customized Optra Color 45 printer/plotter includes special software and is HPGL, PS, and PCL compatible. This custom printer is not available from other sources. The optional tri-port serial port board is installed in the Agilent Optra Color 45 allowing either serial or parallel port mode. The Optra Color 45 replaces the Lexmark 4079, HP 7475, and the HP 7550A plotters.

Self-Test procedure

1 Follow the set up instructions in the printer manual and then plug into ac power.

2 The print display shows Ready, and the green light is on.

3 Click the **Menu** button until TESTS MENU is displayed; and click **Select**.

4 Click the **Menu** button until Print Demo is displayed and click **Select** twice.

A multi-color page should be printed, and the Menu returns to Ready.

Hewlett-Packard DeskJet 5550 Printer

Printer I/O	Centronics Parallel
	Universal serial bus
Printer language	HP PCL 3, PostScript
Printer memory	512 KB standard memory sufficient for full page graphics at 600 dpi
Cartridges	Black and color
Resolution	Black – 600 x 600 dpi
	Color – depends on paper type
Pages per minute	Black – 12 ppm
	Black and color – 10 ppm
Configuration control	Software-controlled

The Hewlett-Packard 5550 features 600 dpi color printing and is software-controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the Hewlett-Packard manual for operating procedures.

There are three buttons in the user interface:

- Power button and light should always be used to turn the printer on and off.

- Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

- Cancel button stops the print task.

- Resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Agilent software does not support two-sided printing.

Hewlett-Packard DeskJet 970Cxi Printer

Printer I/O	Centronics Parallel
	Universal serial bus
	1284-B receptacle
Printer language	HP PCL 3
Printer memory	512 Kbyte standard memory sufficient for full page graphics at 600 dpi
Cartridges	black and color
Resolution	Black – 600 x 600 dpi
	Color – depends on paper type
Pages per minute	Black – 12 ppm
	Black and color – 10 ppm
Configuration control	Software controlled

The Hewlett-Packard 970CXI features 600 dpi color printing and is software-controlled. It has a color cartridge and a black cartridge. The control panel has two switches. Refer to the Hewlett-Packard manual for operating procedures.

There are three buttons in the user interface to control the printer:

- Power button and light should always be used to turn the printer on and off. Using a power strip, surge protector, or a wall-mounted switch to turn on the printer may cause premature printer failure.

- Cancel button stops the print task.

- Resume button and light is used when the light above the resume button is flashing. Press the button to continue printing.

Agilent software does not support two-sided printing.

Hewlett-Packard LaserJet 2300 Printer

Printer I/O	Centronics Parallel, USB port
Printer language	HP PCL 6
Printer memory	4 MB standard memory (expandable to 52 MB)
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per minute	10 ppm
Configuration control	Software controlled
Devicetable entry	LaserJet_600 and LaserJet_600R

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

Self-Test procedure

To print the configuration page, press and release the **GO** (large button at bottom of control panel) and **JOB CANCEL** (button at top of control panel with upside down triangle) buttons simultaneously when the printer is in the ready mode.

Hewlett-Packard LaserJet 2100 Printer

Printer I/O	Centronics Parallel, 1284-B receptacle
	LocalTalk port
Printer language	HP PCL 6
Printer memory	4 MB standard memory (expandable to 52 MB)
Cartridges	black
Resolution	1200 x 1200 dpi
Pages per minute	10 ppm
Configuration control	Software controlled

The Hewlett-Packard LaserJet 2100 features 1200 dpi printing and is software-controlled. The control panel has two switches and two lights. Refer to the Hewlett-Packard manual for operating procedures.

Self-Test procedure

To print the configuration page, press the **GO** button (at bottom of control panel) and **JOB CANCEL** button (at top of control panel with upside down triangle buttons) simultaneously when the printer is in the Ready mode.

Hewlett-Packard Color LaserJet 4550 Printer

Printer I/O	Bidirectional parallel port (requires a "C" connector), Two Enhanced Input/Output (EIO) slots; paper handling accessory port; infrared receiver port. IEEE compliant, 1 open EIO slot, HP JetDirect EIO print server for fast Ethernet 10/100Base-TX in second EIO slot.
	(optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer language	HP PCL 5C, PostScript Level 3 Emulation, HP PCL 6
Printer memory	64 MB standard memory (expandable to 192 MB)
Resolution	600 dpi
Pages per minute	16 ppm (black); 4 ppm (color)
Configuration switches	Expanded control panel

Operation

Set up the printer as described in the Hewlett-Packard manual. Specify the printer as a PostScript printer. On the Name and Type lines in the file /vnmr/devicenames, type PS for a printer and PS_AR for a plotter. In the user's global file, set maxpen=8.

Hewlett-Packard LaserJet 5000 Series Printers

Printer I/O	IEEE 1284-compliant bidirectional parallel, RS-232 9-pin serial, 2 PCI-based EIO slots
Printer language	HP PCL 5e, HP PCL 6, and Postscript Level 2 emulation
Printer memory	4 MB standard memory (expandable to 100 MB)
Resolution	1200 dpi
Pages per minute	16 ppm
Configuration switches	Control panel

Overview

The Hewlett-Packard 5000 provides large format (11 x 17") printing at 16 pages per minute.

The control panel has an LCD display, three LEDs and six buttons.

The LaserJet 5000 features 1200 dpi resolution, but for NMR typical applications the plot lines are too fine. You may even fail to plot a full page at this resolution without expanding the printer memory since a full 11" x 17" page takes up to 32 MBytes of pixel information. Also even in parallel interface applications transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice. For publication quality spectra and reproduction, 300 dpi is a better option since the plot looks darker.

Switching between large and standard formats requires changing the paper size in the printer configuration menu on the LaserJet 5000.

Self-Test procedure

1 Load paper and toner cartridge. Press the **Go** button to turn printer on.

Wait until the printer warms up.

The READY message should be displayed.

2 Press **Menu** until the display reads **INFORMATION MENU**.

3 Press **Item** until the display reads **PRINT CONFIGURATION**.

4 Press **Select** to print the configuration page.

5 The configuration page shows the printer's current configuration.

Operation

Set up as described in the Hewlett-Packard printer manual.

Hewlett-Packard Color Inkjet CP1700 Printer

Printer I/O	Bidirectional parallel port (requires a "C" connector) Two Enhanced Input/Output (EIO) slots Paper handling accessory port Infrared receiver port. USB, IEEE-1284 (parallel), Infrared, and network LIO. (optional) HP JetDirect 600N and 610N (EIO) internal print servers, external print servers, connectivity card
Printer language	HP color Inkjet cp1700: HP PCL 3 enhanced HP color Inkjet cp1700d: HP PCL 3 enhanced HP color Inkjet cp1700ps: HP PCL 3 enhanced
Printer memory	16 megabyte (MB) built-in random access memory (RAM), cannot be upgraded. 4 megabytes (MB) built-in read only memory (ROM), cannot be upgraded
Resolution	1200 x 1200 dpi (black); 2400 x 1200 dpi (color)
Pages per minute	16 ppm (black); 14.5 ppm (color)

Overview

The control panel has an LCD display representing ink levels and printer status. There are also three push buttons to control power on/off, resume, and cancel. The resume and power switches have a LED associated with them.

The CP1700D features 1200 dpi resolution for black and white printing and 2400 dpi for color, but for NMR typical applications the plot lines are too fine. It might not be possible to plot a full page at this resolution without expanding the printer memory because a full 11" x 17" page takes up to 32 Mbytes of pixel information. Also, even in parallel interface applications, transferring data is unacceptably slow. For good plot resolution, 600 dpi is a good choice. For publication quality spectra and reproduction 300 dpi is a better option since the plot looks darker.

Self-Test procedure

1 Load paper, ink tanks, and print heads.

Click the **Power** button to turn printer on.

2 Wait until the printer initializes and reports Ready.

3 Press and hold down the **Resume** button in the control panel for three seconds until the LCD display reports processing Job.

A test page is automatically printed.

Operation

Set up as described in the Hewlett-Packard printer manual.

B   Printers and Plotters Troubleshooting

C
Locator Administration

Restricting User's Data Viewing Privileges in Locator

The system administrator can restrict how files appear in the Locator for each user. An access list controls the data that is visible to the users.

Show the access list

Use these steps to show the Access field in the User Information panel on the right side of the VnmrJ 3.2 Admin interface.

1 Open the **VnmrJ 3.2 Administration** interface, if is not already open.

2 Click the button with the **user's name** to select the user.

3 Open the Users Defaults window:

   a Click **Configure**.

   b Select **Users**.

   c Select **Defaults**.

4 Select the **access** check box under the Show column.

5 Click **OK**.

An Access line appears in the user information panel on the right side of the VnmrJ 3.2 Admin interface.

Access list

The following steps describe how to set up an access list for a user.

1 Select a user account by clicking on the **User's Name** button.

2 Type a space-separated list of users whose files the selected user can access.
For example, if user1 will be allowed to view files for user2, user3, and user99, type: user2 user3 user99.

3 Click **Save User**.

4 Repeat for each user.

Configuration Files

Configuration files for the Locator are contained in the following directories for the different appmode types:

Interface	Directory
Spectroscopy	/vnmr/shuffler
Individual users	$vnmruser/shuffler

Large Database Recommendations

The maximum number of items to display in the Locator can be controlled by setting its value in Systems Settings window.

Do one the following:

1 Select **Edit**.

2 Select **System settings**.

3 Click the **Display/Plot** tab.

4 Type a value for Max # of items to show in Locator.

Setting the value in **Max # of items to show in Locator** higher than 2000 slows down the response of the Locator by filling Locator table with a large number of rows. A value between 1000 and 2000 gives optimal performance. A row is shown with the word Truncated if the database returns more items than the limit. The message indicates that more items returned but are not shown in the Locator to save time.

Use the following guidelines if the database contains more than 10000 items:

• Set the Locator to show only items that match the criteria of the statement as follows:

• Imager Interface

    a Select **Tools**.

    b Select **System settings**.

    c Click the **Display/Plot** tab.

    d Check the box next to Display only matching items in locator.

- Liquids Interface (Spectroscopy):

  a Select **Edit**.

  b Select **System settings**.

  c Click the **Display/Plot** tab.

  d Check the box next to Display only matching items in locator.

    Do not type values in the Locator statement of all, etc.

- Set values in the Locator statement to match 1000 or 2000 items.

- Do not type values in the Locator statement of all, etc.

- Use the File Browser to limit the directory scope. The Locator only matches items that are in and under the directory the browser defines if the File Browser is displayed.

- Set Max # of items to show in Locator between **1000** to **2000**.

Network Database

Several computers running VnmrJ 3.2 can access the same Postgres database server. This way, all of the VnmrJ 3.2 users will have immediate access to data saved on other machines (if the user has access to that data).

This access requires that all computers running in network database mode be mounted to any directories of other computers containing data that is intended to be accessed. The mounts can be hard mounts listed in the vfstab file or automount, but they must be mounted to gain access.

Set the environment variable PGHOST to the host name of the machine to use for the DB server in every user account. The default is the local host. Different users can use different DB servers, or some computers can use their own database server. A computer which is to be a DB server will need the Postgres postmaster daemon running on it. Even if it is running, if PGHOST is set to a remote computer, the remote computer will be used.

Non DB server computers default to network mode DB access by comparing PGHOST with the local host name. Specifying a remote host sets the non DB server computer in network mode. The DB server computer has itself as PGHOST, and the VnmrJ 3.2 administrator on the server computer must create an empty file

/usr/varian/config/NMR_NETWORK_DB

to force it into network mode. Data access from other computers will not work correctly if this is not done. Setting this variable on non server computer will force it into network mode.

The file /usr/varian/config/NMR_NETWORK_DB, if it is used, must be in place before dbsetup is run during installation, or the DB will not be set up correctly.

The attribute 'hostdest' in the database contains the host name where the file actually resides (destination) when a computer is set up for network mode. The attribute

'host_fullpath' contains `hostdest:fullpath` where
`fullpath` is the path as it looks on the machine,
`hostdest`. It does show the mounted path from the current
machine.

Pushing automount relations from a server makes the
following necessary:

VnmrJ 3.2 must be able to translate between the mounted
path and the actual path on the destination computer. It will
first look for a file

```
'/usr/varian/mount_name_table'
```

It only uses this file if it is found. An example of this file is
as follows:

```
# Table of remote system mount names and paths
# One line per entry, Syntax:
#host:direct_path   mount_path
mongoose:/export/home/mongoose_home
voyager:/export/home/home
```

If 'mount_name_table' is not found, it looks in
`'/etc/mnttab'` and in `'/etc/auto_direct'` to get
relationships. If automount relations are pushed from a
server, they will not always be available in these files and
will need to be put into a `'mount_name_table'` file.
Mounts from the `vfstab` file and from the local
`auto_direct` file, should work properly without a
`'mount_name_table'` file.

Changing the UNIX port number is not normally necessary,
but might be done if more than one Postgres daemon is to
run on the system at one time. The port will default to 5432
unless specified otherwise in every user's login file with the
environment variable, PGPORT. It should be possible for
different users (and thus different groups) to use entirely
different database daemons and databases on the same
computer. If PGPORT is set to something other than 5432,
then every user on every computer using that DB server will
need PGPORT set in their accounts.

Database Hints

If the Locator shows Error under the column headings, or if the error message, DataBase contents version is not correct, appears on the bottom of the screen, exit VnmrJ 3.2 and run `dbsetup` in a terminal window.

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